Page 1

```
L30
     ANSWER 6 OF 9
                     HCAPLUS
                               COPYRIGHT 1998 ACS
ΑN
     1996:758983
                   HCAPLUS
DN
     126:31794
     Transition metal catalysts based on bidentate ligands containing
TI
     pyridine or quinoline moiety
     Nagy, Sandor; Krishnamurti, Ramesh; Tyrell,
IN
     John A.; Cribbs, Leonard V.; Cocoman, Mary
PA
     Occidental Chemical Corporation, USA
SO
     PCT Int. Appl., 24 pp.
     CODEN: PIXXD2
PΙ
     WO 9633202 A2
                     961024
DS
         AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP,
         KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, UZ, VN
     RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB,
         GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG
AΙ
     WO 96-US3656
                    960318
PRAI US 95-423232
                    950417
DT
     Patent
LA
     English
IC
          C07F017-00
     ICM
     ICS B01J031-122; C08F010-00
CC
     35-3 (Chemistry of Synthetic High Polymers)
     Section cross-reference(s): 29
     MARPAT 126:31794
ÓS
GΙ
```

$$(R^{1})_{m}$$

$$(R^{1})_{p}$$

$$(R^{1})_{p}$$

$$(R^{1})_{p}$$

$$(R^{1})_{m}$$

Transition metal catalysts for .alpha.-olefin polymn. are characterized by having bidentate ligands contg. pyridine or quinoline moiety and have general structure I and II [Y = O, S, NR, (CR2)nNR, (CR2)nO; R = H, C1-6 alkyl; R' = R, C1-6 alkoxy, C6-16 aryl, halogen, CF3; M = Ti, Zr, Hf; X = halogen, C1-6 alkyl, C1-6 alkoxy, NR2; L = X, cyclopentadienyl, C1-6 alkyl-substituted cyclopentadienyl, indenyl, fluorenyl, III; m = 0-4; n = 1-4, p = 0-3]. Thus polyethylene with Mw/Mn 3.67 and melt flow rate 10.2 was produced by using a catalyst system including 8-quinolinoxytitanium trichloride, which was prepd. from 8-hydroxyquinoline and TiC14, and

- Me aluminoxanes in a molar ratio of Al/Ti = 1074; the catalyst productivity was 167.9 kg/g Ti/h. polymn catalyst olefin alpha; pyridine quinoline ligand transition
- metal catalyst

ST

IT Coordination polymerization catalysts

(transition metal catalysts based on bidentate ligands contg. pyridine or quinoline moiety for .alpha.-olefin polymn.)

IT Methyl aluminoxanes

(transition metal catalysts based on bidentate ligands contg. pyridine or quinoline moiety for .alpha.-olefin polymn.)

IT Linear low-density polyethylenes

(transition metal catalysts based on bidentate ligands contg. pyridine or quinoline moiety for .alpha.-olefin polymn.)

IT 72-80-0 142-08-5, 2-Pyridinone 148-24-3, 8-Hydroxyquinoline,
 reactions 1270-98-0, Cyclopentadienyltitanium trichloride
 7550-45-0, Titanium tetrachloride, reactions 34767-44-7,
 Cyclopentadienylzirconium trichloride

(prepn. of transition metal catalysts based on bidentate ligands contg. pyridine or quinoline moiety)

IT 15614-57-0P 184534-40-5P 184534-41-6P 184534-42-7P 184534-43-8P 184534-44-9P

(transition metal catalysts based on bidentate ligands contg. pyridine or quinoline moiety for .alpha.-olefin polymn.)

IT 9002-88-4P, Polyethylene 25087-34-7P (transition metal catalysts based on bidentate ligands contg. pyridine or quinoline moiety for .alpha.-olefin polymn.)

Page 1 compounds atted

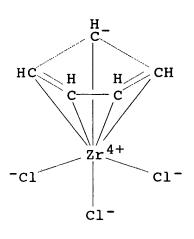
abstracts

14 ANSWERS REGISTRY COPYRIGHT 1998 ACS L31

Zirconium, trichloro(.eta.5-2,4-cyclopentadien-1-yl)- (9CI) IN

C5 H5 Cl3 Zr MF

CI CCS, COM



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):9

14 ANSWERS REGISTRY COPYRIGHT 1998 ACS L31

Titanium, trichloro(5,7-dichloro-2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) IN

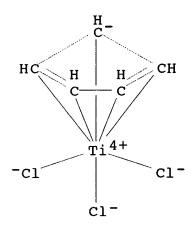
C10 H6 C15 N O Ti

CCS CI

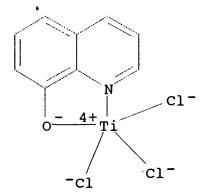
MF

L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS
IN 8-Quinolinol, 5,7-dichloro-2-methyl- (6CI, 7CI, 8CI, 9CI)
MF C10 H7 Cl2 N O
CI COM

L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS
IN Titanium, trichloro(.eta.5-2,4-cyclopentadien-1-yl)- (9CI)
MF C5 H5 Cl3 Ti
CI CCS, COM



L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS
IN Titanium, trichloro(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI)
MF C9 H6 Cl3 N O Ti
CI CCS



L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS

IN Titanium, dichlorobis(2(1H)-pyridinonato-.kappa.O2)-, (T-4)- (9CI)

MF C10 H8 Cl2 N2 O2 Ti

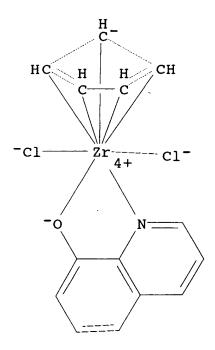
CI CCS

L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS

IN Zirconium, dichloro(.eta.5-2,4-cyclopentadien-1-yl)(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI)

MF C14 H11 Cl2 N O Zr

CI CCS



L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS

IN 2(1H)-Pyridinone (9CI)

MF C5 H5 N O

CI COM

L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS

IN Titanium chloride (TiCl4) (T-4) - (9CI)

MF Cl4 Ti

CI COM

L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS

IN 1-Butene, polymer with ethene (9CI)

ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT

MF (C4 H8 . C2 H4) \times

CI PMS

CM 1

$$H_3C-CH_2-CH=CH_2$$

CM 2

$$H_2C = CH_2$$

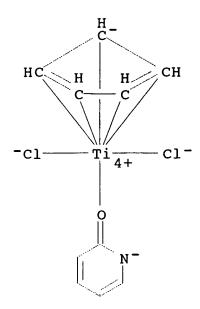
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):9

L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS

IN Titanium, dichloro(.eta.5-2,4-cyclopentadien-1-yl)(2(1H)pyridinonato-.kappa.02)- (9CI)

MF C10 H9 Cl2 N O Ti

CI CCS

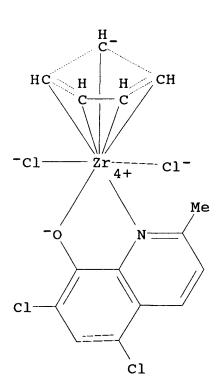


L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS

IN Zirconium, dichloro(.eta.5-2,4-cyclopentadien-1-yl)(5,7-dichloro-2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI)

MF C15 H11 Cl4 N O Zr

CI CCS



L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS IN 8-Quinolinol (7CI, 8CI, 9CI)

L31 14 ANSWERS REGISTRY COPYRIGHT 1998 ACS IN Ethene, homopolymer (9CI) ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT MF (C2 H4)x CI PMS, COM

CM 1

 $H_2C = CH_2$

ALL ANSWERS HAVE BEEN SCANNED

=> file reg

FILE 'REGISTRY' ENTERED AT 14:16:32 ON 04 AUG 1998 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 1998 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 31 JUL 98 HIGHEST RN 209323-09-1 DICTIONARY FILE UPDATES: 3 AUG 98 HIGHEST RN 209323-09-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 14, 1998

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Stereochemical name changes have been adopted and appear in CN's beginning 6/29/30. See the online news message for details.

=> d his

(FILE 'REGISTRY' ENTERED AT 13:15:54 ON 04 AUG 1998) DEL HIS Y ACT RAB659/A

L1STR

L2SCR 1988 OR 1984 OR 2001 OR 1966 OR 1991 OR 1965

L3 SCR 1838

L4SCR 1942

L53550 SEA FILE=REGISTRY SSS FUL L1 AND L2 AND L3 AND L4

FILE 'LREGISTRY' ENTERED AT 13:17:39 ON 04 AUG 1998 L6 STR L1

FILE 'REGISTRY' ENTERED AT 13:22:55 ON 04 AUG 1998 L7 50 S L6 SSS SAM SUB=L5

FILE 'HCAPLUS' ENTERED AT 13:33:38 ON 04 AUG 1998 L8 0 S 126:31794/AN

FILE 'HCAPLUS' ENTERED AT 13:34:20 ON 04 AUG 1998 L9 1 S 1996:758983/AN SEL

L9 1 RN

FILE 'REGISTRY' ENTERED AT 13:34:53 ON 04 AUG 1998

L10 14 S E1-E14

L11 6 S L10 AND M/ELS AND N/ELS

FILE 'HCA' ENTERED AT 13:35:52 ON 04 AUG 1998

L12 3 S L11

```
FILE 'REGISTRY' ENTERED AT 13:36:00 ON 04 AUG 1998
L13
                SCR 1984
L14
              5 S L6 AND L13 SSS SAM SUB=L5
L15
            240 S L5 AND (TI OR ZR OR HF)/ELS
     FILE 'LCA' ENTERED AT 13:40:45 ON 04 AUG 1998
           3028 S CAT# OR CATALY?
L16
           4444 S (POLYMER# OR HOMOPOLYMER# OR COPOLYMER# OR TERPOLYMER#
L17
           3571 S (POLYMERIZ? OR POLYMERIS? OR POLYM# OR CURE# OR CURING#
L18
           4525 S (POLYMER## OR HOMOPOLYMER## OR COPOLYMER## OR TERPOLYME
L19
     FILE 'HCA' ENTERED AT 13:46:37 ON 04 AUG 1998
          40131 S (POLYOLEFIN## OR OLEFIN##) (3A) (L18 OR L19)
L20
           1114 S L5
L21
             92 S L15
L22
          14303 S L20 AND L16
L23
L24
             10 S L21 AND L23
             18 S L22 AND L16
L25
L26
         125753 S POLYOLEFIN## OR OLEFIN##
              9 S L25 AND L26
L27
     FILE 'REGISTRY' ENTERED AT 13:52:29 ON 04 AUG 1998
            126 S L6 AND L13 SSS FUL SUB=L5
L28
                SAV L28 RAB659A/A
     FILE 'HCA' ENTERED AT 13:58:38 ON 04 AUG 1998
L29
             61 S L28
L30
              8 S L29 AND L16
L31
              3 S L29 AND L20
L32
              3 S L29 AND L26
              3 S L31 OR L32
L33
              5 S L12 OR L33
L34
L35
              4 S L30 NOT L34
L36
             7 S (L24 OR L27) NOT (L34 OR L35)
L37
             52 S L29 NOT (L34 OR L35 OR L36)
     FILE 'REGISTRY' ENTERED AT 14:16:32 ON 04 AUG 1998
=> d 15 que stat
```

L1

STR

```
C \times G4 \times N
                    C \times G4 \times O
                                       o∼Ak
@38 39 @40
                    @43 44 @45
                                        @48 49
VAR G1=5/15
VAR G2=0/S/32/35/38-17 40-19/43-17 45-19
VAR G3=X/22/25/28/48
REP G4=(0-5) C
NODE ATTRIBUTES:
CONNECT IS E1 RC AT
                RC AT
CONNECT IS E1
                        29
CONNECT IS E1
                RC AT
                        33
CONNECT IS E1
                RC AT
                        36
CONNECT IS E1
                RC AT
CONNECT IS E1
                RC AT
                        49
DEFAULT MLEVEL IS ATOM
GGCAT
        IS SAT
                 AΤ
                     22
GGCAT
        IS UNS
                 AT
                     25
GGCAT
        IS SAT
                 AT
                     29
GGCAT
        IS SAT
                 AT
                     33
GGCAT
        IS SAT
                 AΤ
                     36
GGCAT
        IS SAT
                 AT
                     37
GGCAT
        IS SAT
                 AT
                     49
DEFAULT ECLEVEL IS LIMITED
```

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 37

STEREO ATTRIBUTES: NONE

SCR 1988 OR 1984 OR 2001 OR 1966 OR 1991 OR 1965 L2

L3 SCR 1838 L4SCR 1942

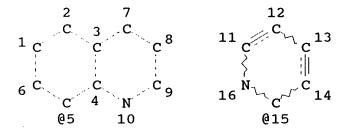
L5 3550 SEA FILE=REGISTRY SSS FUL L1 AND L2 AND L3 AND L4

100.0% PROCESSED 206509 ITERATIONS (2 INCOMPLETE) 3550 ANSWERS

SEARCH TIME: 00.05.00

=> d l15 que stat

L1STR



 $G1 \times G2 \times M \sim G3$ Ak @22 Cb @25 $N \sim Ak$ 17 18 19 20 **@28** 29

N√Ak P-√Ak @32 33 @35 36

37 Ak

 $C \times G4 \times N$ @38 39 @40

 $C \times G4 \times O$ **@43 44 @45**

O√Ak @48 49

VAR G1=5/15

VAR G2=0/S/32/35/38-17 40-19/43-17 45-19

VAR G3=X/22/25/28/48

REP G4=(0-5) C

```
NODE ATTRIBUTES:
CONNECT IS E1
               RC AT
                       22
CONNECT IS E1
                RC AT
                       29
CONNECT IS E1
               RC AT
                       33
CONNECT IS E1
               RC AT
CONNECT IS E1
               RC AT
                       37
CONNECT IS E1
               RC AT
DEFAULT MLEVEL IS ATOM
GGCAT
        IS SAT
                 AT
                     22
        IS UNS
GGCAT
                 AT
                     25
        IS SAT
GGCAT
                 AT
                     29
        IS SAT
                 AT
                     33
GGCAT
GGCAT
        IS SAT
                AΤ
                     36
        IS SAT
GGCAT
                AT
                     37
      IS SAT
                AT
                     49
GGCAT
DEFAULT ECLEVEL IS LIMITED
```

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 37

STEREO ATTRIBUTES: NONE

L2 SCR 1988 OR 1984 OR 2001 OR 1966 OR 1991 OR 1965
L3 SCR 1838
L4 SCR 1942
L5 3550 SEA FILE=REGISTRY SSS FUL L1 AND L2 AND L3 AND L4
L15 240 SEA FILE=REGISTRY L5 AND (TI OR ZR OR HF)/ELS

=> file hca

FILE 'HCA' ENTERED AT 14:17:22 ON 04 AUG 1998
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 1998 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE COVERS 1967 - 1 Aug 1998 (980801/ED) VOL 129 ISS 6

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 134 1-5 cbib abs hitstr hitind

L34 ANSWER 1 OF 5 HCA COPYRIGHT 1998 ACS

128:128339 Syndiotactic polymerization of styrene using titanium-8-hydroxyquinolinate complex/methyl aluminoxane systems. Xu, Xuexiang; Zhou, Nai; Xie, Guanghua (Chinese Academy of Sciences, Institute of Chemistry, Beijing, 100080, Peop. Rep. China).

Gaofenzi Xuebao (6), 746-748 (Chinese) 1997. CODEN: GAXUE9. ISSN: 1000-3304. Publisher: Kexue Chubanshe.

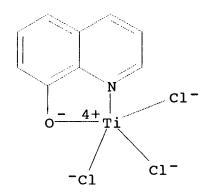
AB Titanium-8-hydroxyquinolinate complexes in combination with Me aluminoxane (MAO) as cocatalyst are highly active towards styrene polymn., giving polymers with high syndiotacticity. The mol.-wt. distribution of polymers is broader, indicating the Ti complexes may be a "multi-site" catalyst.

IT 15614-57-0

(syndiotactic polymn. of styrene using titanium-8-hydroxyquinolinate complex/methylaluminoxane systems as catalysts)

RN 15614-57-0 HCA

CN Titanium, trichloro(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)



CC 35-4 (Chemistry of Synthetic High Polymers)
IT 15614-57-0 16905-40-1 17442-90-9 17500-80-0
(syndiotactic polymn. of styrene using titanium-8-hydroxyquinolinate complex/methylaluminoxane systems as catalysts)

L34 ANSWER 2 OF 5 HCA COPYRIGHT 1998 ACS

128:102528 Transition metal catalyst for the production of olefin polymers. Reichle, Walter Thomas; Karol, Frederick John (Union Carbide Chemicals + Plastics Technology Corp., USA). PCT Int. Appl. WO 9749713 A1 971231, 28 pp. DESIGNATED STATES: W: AU, BR, CA, JP, MX; RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 97-US12236 970625. PRIORITY: US 96-670507 960627.

AB A catalyst compn. for the **polymn**. of **olefins** comprises a bis(hydroxy arom. N ligand) transition metal catalyst precursor and an activating cocatalyst. A catalyst was prepd. by reaction of 2-hydroxypyridine (in PhMe) with n-BuLi (in hexane), then TiCl4 to give a brown slurry (80 .mu.mole Ti/mL). This catalyst, activated with Me aluminoxane, was used to polymd. C2H4 at 65.degree. in 30 min.

IT 201299-99-2 201300-00-7

(transition metal catalyst for prodn. of ${\tt ol}$ fin ${\tt polym}$ rs)

RN 201299-99-2 HCA

CN Zirconium, dichlorobis(2(1H)-pyridinonato-.kappa.O2)-, (T-4)- (9CI) (CA INDEX NAME)

RN 201300-00-7 HCA

CN Zirconium, [[2,2'-bipyridine]-6,6'(1H,1'H)-dionato(2-)-.kappa.06]dichloro- (9CI) (CA INDEX NAME)

IC ICM C07F019-00

ICS C08F004-60; C08F004-602; C08F010-00

CC 35-3 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 67

ST single site polymn catalyst olefin; transition

metal polymn catalyst olefin; metallocene

polymn catalyst olefin; hydroxy heteroarom

nitrogen bound metallocene catalyst; aluminoxane cocatalyst metallocene catalyst **olefin polymn**

IT Methyl aluminoxanes

(cocatalyst; transition metal catalyst for prodn. of olefin polymers)

IT Polymerization catalysts

(hydroxypyridine bound transition metal; transition metal catalyst for prodn. of **olefin polymers**)

IT Metallocenes

(hydroxypyridine bound transition metal; transition metal catalyst for prodn. of olefin polym rs)

IT 7550-45-0, Titanium tetrachloride, uses 10026-11-6, Zirconium tetrachloride 72762-00-6, 2-Hydroxypyridine 201299-99-2

201300-00-7

(transition metal catalyst for prodn. of **ol fin** polymers)

IT 9002-88-4P, Polyethylene 25213-02-9P, Ethylene-1-hexene copolymer (transition metal catalyst for prodn. of **olefin** polymers)

L34 ANSWER 3 OF 5 HCA COPYRIGHT 1998 ACS

126:31794 Transition metal catalysts based on bidentate ligands containing pyridine or quinoline moiety. Nagy, Sandor; Krishnamurti, Ramesh; Tyrell, John A.; Cribbs, Leonard V.; Cocoman, Mary (Occidental Chemical Corporation, USA). PCT Int. Appl. WO 9633202 A2 961024, 24 pp. DESIGNATED STATES: W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, UZ, VN; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 96-US3656 960318. PRIORITY: US 95-423232 950417.

 $(R^{1})_{m}$ $(R^{1})_{p}$ $(R^{1})_{p}$ $(R^{1})_{p}$ $(R^{1})_{p}$ $(R^{1})_{m}$ $(R^{1})_{m}$

Transition metal catalysts for .alpha.-olefin

polymn. are characterized by having bidentate ligands contg.

pyridine or quinoline moiety and have general structure I and II [Y = 0, S, NR, (CR2)nNR, (CR2)nO; R = H, C1-6 alkyl; R' = R, C1-6

alkoxy, C6-16 aryl, halogen, CF3; M = Ti, Zr, Hf; X = halogen, C1-6

alkyl, C1-6 alkoxy, NR2; L = X, cyclopentadienyl, C1-6

alkyl-substituted cyclopentadienyl, indenyl, fluorenyl, III; m =

0-4; n = 1-4, p = 0-3]. Thus polyethylene with Mw/Mn 3.67 and melt

flow rate 10.2 was produced by using a catalyst system including

8-quinolinoxytitanium trichloride, which was prepd. from

8-hydroxyquinoline and TiCl4, and Me aluminoxanes in a molar ratio

of Al/Ti = 1074; the catalyst productivity was 167.9 kg/g Ti/h.

IT 15614-57-0P 184534-40-5P 184534-41-6P 184534-42-7P 184534-43-8P 184534-44-9P

GI

(transition metal catalysts based on bidentate ligands contg.

pyridine or quinoline moiety for .alpha.-olefin
polymn.)

RN 15614-57-0 HCA

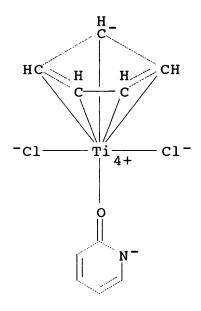
CN Titanium, trichloro(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)

RN 184534-40-5 HCA

CN Titanium, dichlorobis(2(1H)-pyridinonato-.kappa.O2)-, (T-4)- (9CI) (CA INDEX NAME)

RN 184534-41-6 HCA

CN Titanium, dichloro(.eta.5-2,4-cyclopentadien-1-yl)(2(1H)-pyridinonato-.kappa.O2)- (9CI) (CA INDEX NAME)

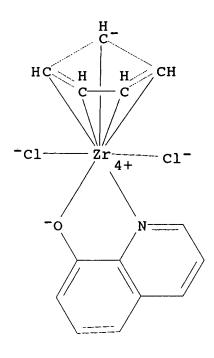


RN 184534-42-7 HCA

CN Titanium, trichloro(5,7-dichloro-2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8) - (9CI) (CA INDEX NAME)

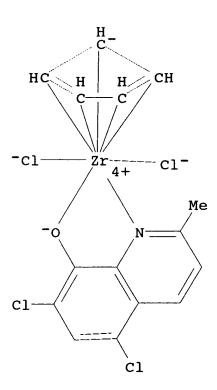
RN 184534-43-8 HCA

CN Zirconium, dichloro(.eta.5-2,4-cyclopentadien-1-yl)(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)



RN 184534-44-9 HCA

CN Zirconium, dichloro(.eta.5-2,4-cyclopentadien-1-yl)(5,7-dichloro-2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)



```
IC
     ICM C07F017-00
     ICS B01J031-122; C08F010-00
     35-3 (Chemistry of Synthetic High Polymers)
CC
     Section cross-reference(s): 29
     polymn catalyst olefin alpha; pyridine quinoline
ST
     ligand transition metal catalyst
IT
     Coordination polymerization catalysts
        (transition metal catalysts based on bidentate ligands contg.
        pyridine or quinoline moiety for .alpha.-olefin
      polymn.)
IT
     Methyl aluminoxanes
        (transition metal catalysts based on bidentate ligands contg.
        pyridine or quinoline moiety for .alpha.-olefin
      polymn.)
IT
     Linear low-density polyethylenes
        (transition metal catalysts based on bidentate ligands contg.
        pyridine or quinoline moiety for .alpha.-olefin
      polymn.)
IT 15614-57-0P 184534-40-5P 184534-41-6P
   184534-42-7P 184534-43-8P 184534-44-9P
        (transition metal catalysts based on bidentate ligands contg.
        pyridine or quinoline moiety for .alpha.-olefin
      polymn.)
     9002-88-4P, Polyethylene
                                25087-34-7P
IT
        (transition metal catalysts based on bidentate ligands contg.
        pyridine or quinoline moiety for .alpha.-olefin
      polymn.)
    ANSWER 4 OF 5 HCA COPYRIGHT 1998 ACS
125:143539 Olefin polymerization catalyst and
     manufacture of polyolefins using the same with narrow
     molecular weight distribution. Nitto, Yu; Kaneshima, Tokitaka;
     Aoki, Toshiya (Asahi Kasei Kogyo Kabushiki Kaisha, Japan).
                                                                 PCT Int.
     Appl. WO 9618658 A1 960620, 164 pp. DESIGNATED STATES: W:
     US; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT,
          (Japanese). CODEN: PIXXD2. APPLICATION: WO 95-JP2558 951213.
     PRIORITY: JP 94-308729 941213; JP 94-308730 941213.
AΒ
    An olefin polymn. catalyst contains a transition
    metal compd. composed of .gtoreg.1 transition metal selected from
     Ti, Zr and Hf and .gtoreq.2 ligands, one of which has a
     cyclopentadienyl skeleton and the other(s) of which is a monovalent
    bidentate anionic ligand contq. an element selected from O, S, Se
     and Te and one selected from N, S, Se and Te as coordinating atoms
    through which the ligand is coordinated with the transition metal,
     one of the latter ligands being optionally bonded to the group
    having a cyclopentadienyl skeleton through a crosslinking group; and
```

a process for efficiently prepg. an **ol fin** homo- or **copolym r** with this catalyst. The polymn. of one or more **olefins** with the above catalyst can give a homopolymer

having a narrow mol. wt. distribution or a copolymer having a narrow

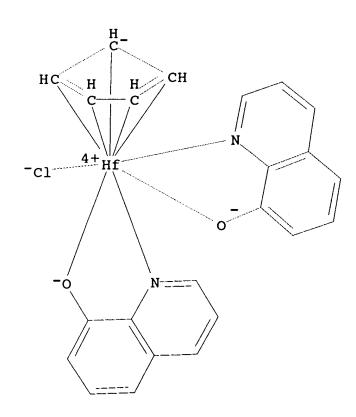
mol. wt. distribution and a uniform compn., and these homo- and copolymers are excellent in impact strength, stress cracking resistance, transparency, heat sealability at low temp. and blocking resistance and have low stickiness and extractible content. Ethylene was polymd. in the presence of methylaluminoxane and (pentamethylcyclopentadienyl)tris(dimethyldithiocarbamato)zirconium to give polyethylene with Mw 565,000 and Mw/Mn 2.56.

IT 33291-90-6P 180079-17-8P 180079-21-4P 180079-22-5P 180079-23-6P 180079-29-2P 180079-31-6P

(catalysts for **polyolefins** using the same with narrow mol. wt. distribution)

RN 33291-90-6 HCA

CN Hafnium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)



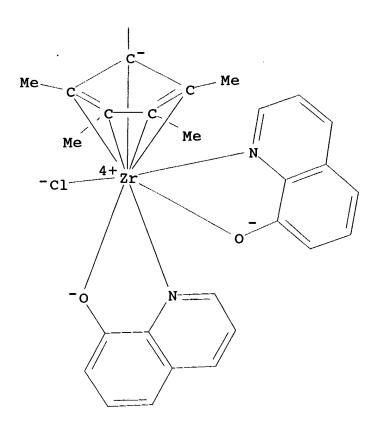
RN 180079-17-8 HCA

CN Zirconium, chloro[(1,2,3,4,5-.eta.)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]bis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

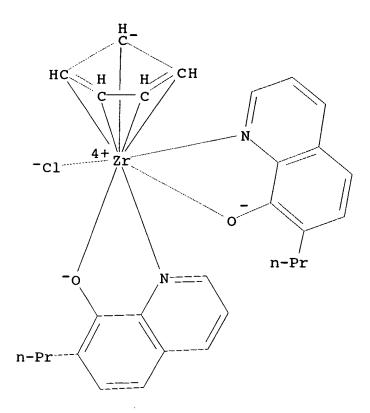
PAGE 1-A

Me |

PAGE 2-A



RN 180079-21-4 HCA
CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(7-propyl-8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)



RN 180079-22-5 HCA
CN Zirconium, [(1,2,3,4,5-.eta.)-1-butyl-2,4-cyclopentadien-1-yl]chlorobis(5-chloro-7-iodo-8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

PAGE 1-A

n-Bu

PAGE 2-A

PAGE 3-A

cl

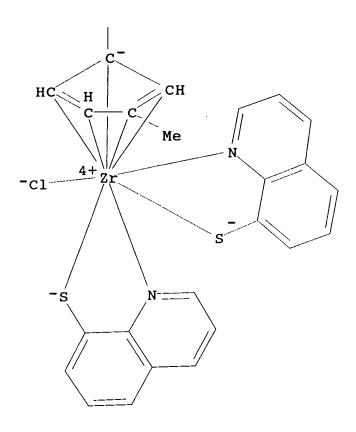
RN 180079-23-6 HCA

CN Zirconium, chloro[(1,2,3,4,5-.eta.)-1,3-dimethyl-2,4-cyclopentadien-1-yl]bis(8-quinolinethiolato-N1,S8)- (9CI) (CA INDEX NAME)

PAGE 1-A

Me

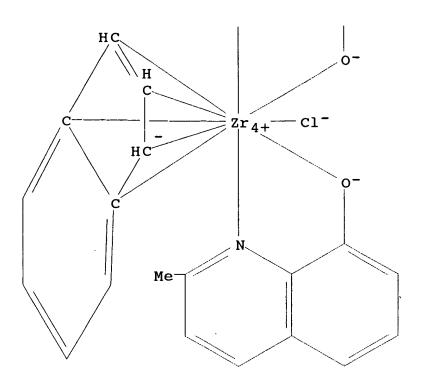
PAGE 2-A



RN 180079-29-2 HCA
CN Zirconium, chloro[(1,2,3,3a,7a-.eta.)-1H-inden-1-yl]bis(2-methyl-8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

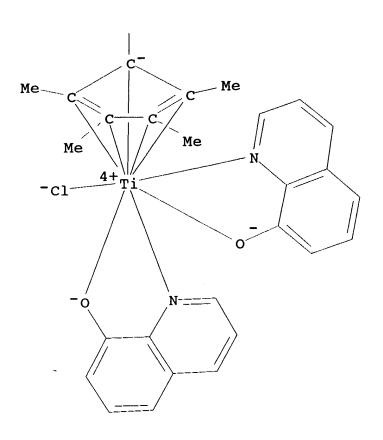


RN 180079-31-6 HCA
CN Titanium, chloro[(1,2,3,4,5-.eta.)-1,2,3,4,5-pentamethyl-2,4cyclopentadien-1-yl]bis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

PAGE 1-A

Me

PAGE 2-A



```
IC
     ICM C08F004-642
          C08F004-645; C08F010-00; C08F012-08; C08F032-00; C08F036-00
     35-3 (Chemistry of Synthetic High Polymers)
CC
     Section cross-reference(s): 67
     transition metal complex olefin polymn catalyst;
ST
     ethylene hexene polymn catalyst; octene ethylene polymn catalyst
     Polymerization catalysts
IT
        (olefin polymn. catalyst and manuf. of
     polyolefins using the same with narrow mol. wt.
        distribution)
IT
     Alkenes
        (polymers, olefin polymn. catalyst
        and manuf. of polyolefins using the same with narrow
        mol. wt. distribution)
IT
     146355-12-6, Tris(pentafluorophenyl)borate
        (catalysts for polyolefins using the same with narrow
        mol. wt. distribution)
                               66200-00-8P
                                              74822-09-6P
                 65554-57-6P
IT 33291-90-6P
                                                   180078-77-7P
     110509-37-0P
                    137657-29-5P
                                   180078-76-6P
     180078-78-8P
                    180078-79-9P
                                   180078-80-2P
                                                   180078-81-3P
                                   180078-88-0P
                                                   180078-89-1P
     180078-82-4P
                    180078-87-9P
                                                   180078-95-9P
                                   180078-93-7P
                    180078-91-5P
     180078-90-4P
```

180078-97-1P

180078-96-0P

180078-99-3P

180079-00-9P

```
180079-03-2P
                                                  180079-04-3P
    180079-01-0P
                    180079-02-1P
                    180079-08-7P
                                   180079-09-8P
                                                  180079-10-1P
    180079-06-5P
     180079-11-2P
                    180079-12-3P
                                   180079-14-5P
                                                  180079-15-6P
    180079-16-7P 180079-17-8P
                                 180079-18-9P
                                                180079-19-0P
     180079-20-3P 180079-21-4P 180079-22-5P
  180079-23-6P
                  180079-24-7P
                                 180079-25-8P
                                                180079-26-9P
                    180079-28-1P 180079-29-2P
                                                180079-30-5P
     180079-27-0P
                                                180079-34-9P
  180079-31-6P
                  180079-32-7P
                                 180079-33-8P
     180079-35-0P
                    180079-36-1P
                                   180079-37-2P
                                                  180079-38-3P
     180079-40-7P
                    180079-41-8P
                                   180079-42-9P
                                                  180079-44-1P
     180079-45-2P
                    180079-46-3P
                                   180079-47-4P
                                                  180079-48-5P
        (catalysts for polyolefins using the same with narrow
       mol. wt. distribution)
    9002-88-4P, Polyethylene
                                25213-02-9P
                                              26221-73-8P
IT
        (catalysts for polyolefins using the same with narrow
       mol. wt. distribution)
    135181-14-5P
                    180078-84-6P
ĬΤ
        (catalysts for polyolefins using the same with narrow
       mol. wt. distribution)
IT
    75-77-4, Trimethylsilyl chloride, reactions
                                                   96-80-0,
    2-Diisopropylaminoethanol
                                 122-98-5, 2-Phenylaminoethanol
     128-04-1, Sodium dimethyldithiocarbamate
                                                130-16-5,
    5-Chloro-8-quinolinol
                             130-26-7, 5-Chloro-7-iodo-8-quinolinol
                140-90-9, Sodium O-ethylxanthate
                                                   141-33-3
    140-89-6
    8-Quinolinol, reactions
                              491-33-8, 8-Quinolinethiol
                                                            555-24-8,
                      586-98-1, 2-Pyridinemethanol
    Phenoxylithium
                                                     643-62-9,
                   826-81-3, 2-Methyl-8-quinolinol
    9-Acridinol
                                                     865-34-9,
    Methoxylithium
                      872-71-9
                                 1068-22-0, Ammonium 0,0'-
    diethyldithiophosphate
                             1085-35-4
                                          1271-19-8,
    Bis(cyclopentadienyl)titanium dichloride
                                                1470-61-7, Silver
    diethyldithiocarbamate 2044-73-7, 2-Pyridinemethanethiol
                 3743-22-4, 2-Dimethylaminophenol
                                                    4092-82-4, Sodium
                                  4787-77-3, 2-Pyrrolidinophenol
    diisopropyldithiocarbamate
    12116-66-4, Bis(cyclopentadienyl)hafnium dichloride
                                                           12129-06-5,
     (Pentamethylcyclopentadienyl)titanium trichloride
                                                         12148-49-1,
    Bis(indenyl)zirconium dichloride
                                       14159-57-0
                                                     18087-24-6,
    2-Dimethylaminothiophenol
                               18938-33-5, Sodium
    dibutyldiselenocarbamate
                                18992-87-5, Sodium dimethylthiocarbamate
     23504-11-2
                  42508-74-7, 4-Methyl-2-pyridinemethanol
                                                            50742-62-6
                              67715-76-8
     54769-08-3
                  66542-75-4
                                           73364-10-0,
    Bis(butylcyclopentadienyl)zirconium dichloride
                                                      75181-07-6,
     (Pentamethylcyclopentadienyl)zirconium trichloride
                                                          81376-81-0
                                                             180078-85-7
    82387-86-8
                  102439-95-2
                                125542-03-2
                                              180078-83-5
                   180078-92-6
                                                              180079-05-4
     180078-86-8
                                 180078-94-8
                                               180078-98-2
     180079-07-6
                   180079-13-4
                                 180079-39-4
                                               180079-43-0
        (catalysts for polyolefins using the same with narrow
        mol. wt. distribution)
```

Reactions of 8-quinolinol with covalent halides.

and titanium(IV) halides. Frazer, Malcolm J.; Rimmer, B. (Northern

ANSWER 5 OF 5 HCA COPYRIGHT 1998 ACS

L34

68:39433

Polytech., London, Engl.). J. Chem. Soc. A (1), 69-74 (English) 1968. CODEN: JCSIAP.

The adducts MX4.20XH (M = Ti or Sn, X = F, Br, and I) are formed AB when 8-quinolinol (OXH) (2 moles) in CHCl3 or tetrahydrofuran is added to the appropriate tetrahalide; with M = Si or Ge, however, adducts are not formed but there is loss of hydrogen halide and pptn. of the dihalodi-8-quinolinolato-metal MX2OX2. The 1:2 adducts, either by the action of heat (X = F, Br, and I), or by the addn. of excess of 8-quinolinol (X = Br and I) give the corresponding MX20X2. The dihalodi-8-quinolinolatotitanium compds. with excess 8-quinolinol give TiXOX3 in which Ti is probably Iodotri-8-quinolinolatotitanium heptacoordinate for X = F and Br. is a 1:1 electrolyte. The trichloro-8-quinolinolato-metals, MCl3OX (M = Ti and Sn), form adducts with 8-quinolinol and with pyridine, and probably contain a pentacoordinate metal atom.

IT 15614-57-0P

(prepn. of)

RN 15614-57-0 HCA

CN Titanium, trichloro(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)

CC 27 (Heterocyclic Compounds (One Hetero Atom)) IT 15523-67-8P 15523-68-9P **15614-57-0P** 16862-11-6P 16880-55-0P 16880-56-1P 16905-16-1P 16905-18-3P 16905-19-4P 16905-20-7P 16905-22-9P 16905-23-0P 16905-24-1P 16905-21-8P 16905-25-2P 16905-26-3P 16905-27-4P 16905-28-5P 16905-30-9P 16905-34-3P 16905-35-4P 16905-31-0P 16905-32-1P 16905-33-2P 16905-39-8P 16905-40-1P 16905-41-2P 16905-42-3P 16905-43-4P 16905-44-5P 17211-42-6P 17211-44-8P 17211-45-9P 17211-46-0P 20471-44-7P 20471-45-8P 18904-87-5P 20471-43-6P 17409-65-3P 20471-46-9P 20471-47-0P 20471-48-1P 20471-49-2P 20471-50-5P 21254-84-2P

=> d 135 1-4 cbib abs hitstr hitind

(prepn. of)

L35 ANSWER 1 OF 4 HCA COPYRIGHT 1998 ACS

128:300202 Catalytic activity of titanium alkoxy derivatives in alcoholysis of ethoxysilanes. Khonina, T. G.; Kochneva, N. A.; Suvorov, A. L. (Ural Division, Institute of Organic Synthesis, Russian Academy of Sciences, Yekaterinburg, Russia). Russ. J. Gen. Chem., 67(1), 79-82 (English) 1997. CODEN: RJGCEK. ISSN: 1070-3632. Publisher: MAIK Nauka/Interperiodica Publishing.

Titanium tetraalkooxides, regardless of their structure, are effective catalysts for alcoholysis of ethoxysilanes.

Titanium alkoxychlorides demonstrate the highest catalytic activity, whereas the catalytic activity of coordination-satd. titanium compds. is the lowest. The influence of the catalyst nature on its activity is analyzed.

IT 206053-84-1

(catalytic activity of titanium alkoxy derivs. in alcoholysis of ethoxysilanes)

RN 206053-84-1 HCA

CN Titanium, dibutoxy(8-quinolinolato-.kappa.N1,.kappa.O8)-, (T-4)- (9CI) (CA INDEX NAME)

CC 67-2 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)

ST titanium alkoxy deriv catalyst alcoholysis ethoxysilane

IT Alcoholysis catalysts

Alcoholysis kinetics

(catalytic activity of titanium alkoxy derivs. in alcoholysis of ethoxysilanes)

546-68-9, Titanium tetraisopropoxide 1070-10-6 1790-25-6 IT 3087-36-3, Titanium tetraethoxide 3087-37-4, Titanium tetrapropoxide 3087-39-6, Titanium tetra-tert-butoxide 3112-68-3 3374-12-7, Titanium tetra-sec-butoxide 4200-76-4 5593-70-4, Titanium tetrabutoxide 7393-49-9 7441-92-1 25902-23-2 206053-82-9 206053-84-1 83328-25-0

(catalytic activity of titanium alkoxy derivs. in alcoholysis of ethoxysilanes)

IT 78-07-9 78-10-4 78-62-6 2031-67-6

(catalytic activity of titanium alkoxy derivs. in alcoholysis of ethoxysilanes)

IT 1591-02-2P 4766-57-8P 5581-68-0P 17957-38-9P (catalytic activity of titanium alkoxy derivs. in

alcoholysis of ethoxysilanes)

- L35 ANSWER 2 OF 4 HCA COPYRIGHT 1998 ACS
- 127:149211 Synthesis, Structures, Bonding, and Ethylene Reactivity of Group 4 Metal Alkyl Complexes Incorporating 8-Quinolinolato Ligands. Bei, Xiaohong; Swenson, Dale C.; Jordan, Richard F. (Department of Chemistry, University of Iowa, Iowa City, IA, 52242, USA). Organometallics, 16(15), 3282-3302 (English) 1997. CODEN: ORGND7. ISSN: 0276-7333. OTHER SOURCES: CJACS-IMAGE; CJACS. Publisher: American Chemical Society.
- This contribution describes the synthesis, structures, bonding, and AB reactivity of neutral (Ox)2MR2 and cationic (Ox)2MR+ zirconium and hafnium alkyl complexes which contain substituted 8-quinolinolato ligands (Ox- = 2-Me-8-quinolinolato, MeOx-, 2; 2-Me-5, 7-Br2-8quinolinolato, MeBr2Ox-, 3). Alkane elimination and halide displacement reactions provide routes to (MeOx)2ZrR2 (9a, R = CH2Ph; 9b, R = CH2CMe3; 9c, R = CH2SiMe3), (MeOx) 2Hf(CH2Ph) 2 (10a), (MeBr2Ox) 2ZrR2 (11a, R = CH2Ph; 11b, R = CH2CMe3),(MeBr2Ox)2Hf(CH2Ph)2 (14a), (MeOx)2ZrCl2 (15), (MeBr2Ox)2ZrCl2 (16), and (MeBr2Ox)2Zr(NMe2)2 (17). The reaction of 16, 17, or (MeBr2Ox) 4Zr with AlMe3 yields (MeBr2Ox) AlMe2 (18). An x-ray crystallog. anal. shows that in the solid state 9a adopts a distorted octahedral structure with a trans-0, cis-N, cis-R ligand arrangement and that one of the benzyl ligands is bonded in an Soln. NMR data are consistent with this structure .eta.2-fashion. and establish that exchange of the distorted and normal benzyl ligands is rapid on the NMR time scale. Soln. NMR data for the other (Ox) 2MR2 complexes are consistent with analogous octahedral, trans-O, cis-N, cis-R structures for these species. Variable-temp. NMR studies establish that (Ox)2MR2 complexes undergo inversion of metal configuration (i.e., .LAMBDA./.DELTA. isomerization, racemization) on the NMR time scale at elevated temps. (.DELTA.G.thermod. (racemization) = 15-18 kcal/mol). Thermolysis of 11a results in migration of a benzyl ligand from Zr to C2 of a MeBr2Ox- ligand, yielding (MeBr2Ox)(2-Me-2-CH2Ph-5,7-Br2-Ox)ZrCH2Ph (19) as a single diastereomer. Reaction of 9a or 9b with [HNMe2Ph][B(C6F5)4] yields the base-free cationic complexes [(MeOx)2Zr(R)][B(C6F5)4] (20a, R = CH2Ph; 20b, R = CH2CMe3), while the corresponding reaction of 11a yields the labile amine adduct [(MeBr2Ox)2Zr(CH2Ph)(NMe2Ph)][B(C6F5)4] (21a). The reaction of [HNMePh2][B(C6F5)4] with the appropriate (Ox)2M(CH2Ph)2 complex yields 20a, [(MeOx)2Hf(CH2Ph)][B(C6F5)4] (22a), or [(MeBr2Ox)2M(CH2Ph)][B(C6F5)4] (23a, M = Zr; 24a, M = Hf). An x-ray crystallog. anal. establishes that the cation of 23a adopts a square pyramidal structure with a highly distorted (.eta.2) benzyl ligand in the apical site and a trans-O, trans-N ligand arrangement in the basal sites, and NMR studies show that 23a and 24a adopt analogous structures in soln. In contrast, NMR studies establish that 20a, 20b, and 22a, which contain the more strongly electron-donating MeOx- ancillary ligand, adopt distorted square pyramidal structures with an apical-O, cis-N ligand arrangement which allows max. O-M

.pi.-donation. The reactions of 23a or 24a with PMe3 yield the adducts [(MeBr2Ox)2M(CH2Ph)(PMe3)][B(C6F5)4] (25a, M = Zr; 26a, M = Hf), which adopt trans-O, cis-N, cis-benzyl/PMe3 structures analogous to those of the (Ox)2MX2 complexes. The (MeBr2Ox)2M(.eta.2-CH2Ph)+ cations 23a and 24a exhibit moderate ethylene polymn. activity, while the MeOx- analogs 20a and 20b are inactive.

IT 193351-79-0P 193352-10-2P 193352-12-4P

(prepn. of)

RN 193351-79-0 HCA

CN Zirconium, bis(5,7-dibromo-2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)bis(N-methylmethanaminato)-, (OC-6-13)- (9CI) (CA INDEX NAME)

RN 193352-10-2 HCA

CN Zirconium(1+), (2,2-dimethylpropyl)bis(2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)-, (SP-5-31)-, tetrakis(pentafluorophenyl)borate (1-) (9CI) (CA INDEX NAME)

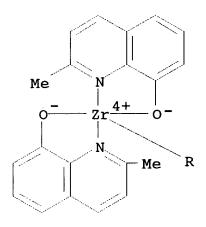
CM 1

CRN 193352-09-9

CMF C25 H27 N2 O2 Zr

CCI CCS

CDES 7:SP-5-31



$$\begin{array}{c} \text{R} & \underline{\hspace{0.5cm}} \text{CH}_2 \underline{\hspace{0.5cm}} \text{CMe}_3 \end{array}$$

CM 2

CRN 47855-94-7

CMF C24 B F20

CCI CCS

RN 193352-12-4 HCA
CN Hafnium(1+), bis(5,7-dibromo-2-methyl-8-quinolinolato.kappa.N1,.kappa.O8)(N,N-dimethylbenzenamine)(phenylmethyl)-,
(OC-6-13)-, tetrakis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 193352-11-3 CMF C35 H30 Br4 Hf N3 O2 CCI CCS CDES 7:OC-6-13

PAGE 2-A

CM 2

CRN 47855-94-7 CMF C24 B F20

cci ccs

IT 193351-78-9P 193352-02-2P

(synthesis, structures, bonding, and ethylene polymn. activity of Group 4 metal alkyl complexes incorporating quinolinolato ligands)

RN 193351-78-9 HCA

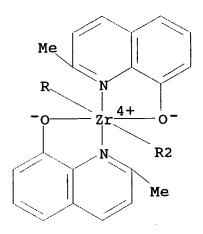
CN Zirconium, dichlorobis(5,7-dibromo-2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)-, (OC-6-33)- (9CI) (CA INDEX NAME)

RN 193352-02-2 HCA

CN Zirconium, bis(2,2-dimethylpropyl)bis(2-methyl-8-quinolinolato-

.kappa.N1,.kappa.O8)-, (OC-6-13)- (9CI) (CA INDEX NAME)

PAGE 1-A



$$_{\text{Me}_3\text{C}}$$
 $_{\text{R}}^{\text{H}_2}$

PAGE 2-A

IT 193351-86-9P

(synthesis, structures, bonding, and ethylene polymn. activity of Group 4 metal alkyl complexes incorporating quinolinolato ligands)

RN 193351-86-9 HCA

CN Zirconium(1+), bis(5,7-dibromo-2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)(N,N-dimethylbenzenamine)(phenylmethyl)-, (OC-6-13)-, tetrakis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 193351-85-8 CMF C35 H30 Br4 N3 O2 Zr CCI CCS

CDES 7:0C-6-13

PAGE 2-A

CM2

47855-94-7 CRN

C24 B F20

CMF CCI CCS

IT 193351-77-8P 193352-06-6P

(synthesis, structures, bonding, and ethylene polymn. activity of Group 4 metal alkyl complexes incorporating quinolinolato ligands)

RN 193351-77-8 HCA

CN Zirconium, dichlorobis(2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)-, (OC-6-33)- (9CI) (CA INDEX NAME)

RN 193352-06-6 HCA

CN Zirconium, bis(5,7-dibromo-2-methyl-8-quinolinolato-.kappa.N1,.kappa.O8)bis(2,2-dimethylpropyl)-, (OC-6-13)- (9CI) (CA INDEX NAME)

PAGE 2-A

CC 29-10 (Organometallic and Organometalloidal Compounds) Section cross-reference(s): 22, 35, 67, 75

zirconium hafnium alkyl quinolinolato complex prepn; cationic zirconium hafnium alkyl quinolinolato prepn; ethylene polymn catalyst quinolinolato zirconium hafnium; FMO quinolinolato zirconium methyl complex; crystal structure benzylzirconium quinolinolato cationic complex; mol structure benzylzirconium quinolinolato cationic complex; isomerization kinetics benzylzirconium benzylhafnium quinolinolato complex; racemization kinetics zirconium hafnium quinolinolato alkyl

TT Polymerization catalysts
(synthesis, structures, bonding, and ethylene polymn. activity of
Group 4 metal alkyl complexes incorporating quinolinolato
ligands)

- IT 9002-88-4P 193351-75-6P **193351-79-0P** 193351-80-3P 193351-81-4P **193352-10-2P 193352-12-4P** (prepn. of)
- IT 193351-78-9P 193352-02-2P

ligands)

(synthesis, structures, bonding, and ethylene polymn. activity of Group 4 metal alkyl complexes incorporating quinolinolato ligands)

193351-72-3P 193351-83-6P **193351-86-9P** 193351-89-2P 193351-94-9P 193351-97-2P 193352-00-0P

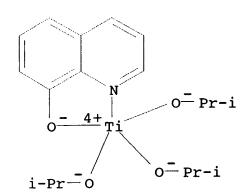
(synthesis, structures, bonding, and ethylene polymn. activity of Group 4 metal alkyl complexes incorporating quinolinolato ligands)

- IT 160883-74-9P 193351-70-1P 193351-77-8P 193352-04-4P
 - 193352-06-6P
 (synthesis, structures, bonding, and ethylene polymn. activity of Group 4 metal alkyl complexes incorporating quinolinolato
- L35 ANSWER 3 OF 4 HCA COPYRIGHT 1998 ACS
- 114:103008 Catalysts for the preparation of alternating polyesters from epoxides and cyclic anhydrides. Bagrel, Valerie; Garapon, Jacques; Touet, Remi; Huet, Catherine; Damin, Bernard (Institut Francais du Petrole, Fr.; Air Liquide, Societe Anon. pour l'Etude et l'Exploitation des Procedes Georges Claude; Elf France). Eur. Pat. Appl. EP 387119 A2 900912, 17 pp. DESIGNATED STATES: R: AT, BE, CH, DE, ES, FR, GB, IT, LI, LU, NL, SE. (French). CODEN: EPXXDW. APPLICATION: EP 90-400490 900221. PRIORITY: FR 89-3140
- The Ti complexes Ti(OR1)m(OR2)n(OR3)pLq (R1-3 = hydrocarbyl; L = N compd.; m, n, p = 0 or 1; Q = 1-4; m + n + p + q = 4) are catalysts for the alternating polymn. of epoxides with cyclic anhydrides. Stirring maleic anhydride 14.7, decycloxirane 27.6, PhC12H25 7.4, PhMe 17.6, and tributoxy(8-quinolinato)titanium 0.62 g at 100.degree. for 6 h gave a 95 and 90% conversion of epoxide and anhydride, resp., to a polyester with no.-av. mol. wt. 7500, with little homopolymn. of the epoxide.
- IT 14843-25-5, Tributoxy(8-quinolinolato)titanium 131479-76-0

(catalysts, for alternating polymn. of epoxides with anhydrides)

- RN 14843-25-5 HCA
- CN Titanium, tributoxy(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

RN 131479-76-0 HCA CN Titanium, tris(2-propanolato)(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)



IC ICM C08G063-42

ICS C08G063-58

CC 35-3 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 67
ST catalyst polymn epoxide anhydride; titanium chelate

catalyst polymn; quinolinol chelate titanium

catalyst; polyester manuf epoxide anhydride; maleic

anhydride copolymer epoxide; decycloxirane copolymer anhydride

IT Polyesters, preparation

(manuf. of, by alternating polymn. of epoxides with cyclic anhydrides, catalysts for)

IT Polymerization catalysts

(alternating, titanium nitrogen compd. complexes, for epoxides with cyclic anhydrides)

IT Anhydrides

(cyclic, polymers, with epoxides, manuf. of, catalysts for)

IT Epoxides

(polymers, with cyclic anhydrides, manuf. of, catalysts

for)

IT 14843-25-5, Tributoxy(8-quinolinolato)titanium 40506-24-9 55235-58-0 131479-76-0 131479-77-1 132529-98-7 (catalysts, for alternating polymn. of epoxides with anhydrides)

IT 131479-70-4P 131479-71-5P 131479-72-6P 131552-41-5P 131552-44-8P 131552-50-6P (manuf. of, catalysts for)

L35 ANSWER 4 OF 4 HCA COPYRIGHT 1998 ACS

84:60078 Polymerization of butadiene on alkyl-o-titanatetriisobutylaluminum systems. Monakov, Yu. B.; Rafikov, S. R.; Ivanova, A. M.; Panasenko, A. A.; Tolstikov, G. A.; Pozdeeva, A. A.; Zaev, E. E.; Lukmanova, R. Z.; Igoshkina, G. S. (Bashk. Filial, Inst. Khim., Ufa, USSR). Vysokomol. Soedin., Ser. A, 17(12), 2631-6 (Russian) 1975. CODEN: VYSAAF.

The polymn. of butadiene (I) in the presence of the binary catalytic system composed of triisobutylaluminum [100-99-2] and Ti(OR)4 (where R = Bu-C9H19) at 22.degree. showed that the highest polymn. rate was reached in the presence of Ti(OBu)4 [5593-70-4]-(iso-Bu)3Al at a ratio of Al:Ti = 8:1. The microstructure of polybutadiene [9003-17-2] was independent of monomer conversion or Al:Ti ratio. The ir spectra of the catalytic system contg. I suggest that the reactive polymn. sites are Ti(III) compds.

IT 17034-82-1

(catalysts, contg. triisobutylaluminum, for polymn. of butadiene)

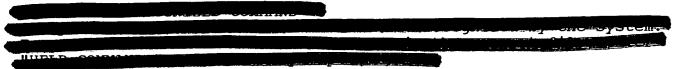
RN 17034-82-1 HCA

CN Titanium, dibutoxybis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

CC 35-4 (Synthetic High Polymers)

butadiene polymn binary catalyst; titanium organo catalyst polymn; aluminum organo catalyst polymn; kinetics polymn butadiene catalyst

```
ΙT
    Polymerization catalysts
        (alkyl titanate-triisobutylaluminum, for butadiene)
TI
     100-99-2, uses and miscellaneous
        (catalysts, contg. alkyl titanates, for polymn. of
        butadiene)
                                          7360-52-3
                             6167-42-6
                                                      10585-24-7
IT
     1790-25-6
                 5593-70-4
     16902-59-3 17034-82-1
                             22063-06-5
        (catalysts, contg. triisobutylaluminum, for polymn. of
        butadiene)
     9003-17-2P
IT
        (prepn. of, catalysts for)
```



=> d 136 1-7 cbib abs hitstr hitind

L36 ANSWER 1 OF 7 HCA COPYRIGHT 1998 ACS

128:212149 A pyridine dialkoxide titanium dichloride complex. Synthesis and molecular structure of 2,6-bis(2,2-diphenyl-2-trimethylsilyloxyethyl)pyridine. Mack, Helmut; Eisen, Moris S. (Department of Chemistry, Technion-Israel Institute of Technology, Haifa, 32000, Israel). J. Chem. Soc., Dalton Trans. (6), 917-922 (English) 1998. CODEN: JCDTBI. ISSN: 0300-9246. Publisher: Royal Society of Chemistry.

Reaction of 2,6-dimethylpyridine with 2 equiv of LiBu followed by addn. of 2 equiv of benzophenone and the consecutive reaction with 2 equiv of SiMe3Cl afforded the doubly functionalized 2,6-bis(2,2-diphenyl-2-trimethylsilyloxyethyl)pyridine L. The structure of L was detd. by an x-ray diffraction study. Reaction of either a doubly lithiated intermediate or the corresponding silylated ligand L with TiCl4 afforded a pyridine dialkoxide titanium dichloride complex TiL'Cl2 (LH2 = 2,6-pyridinebis(2,2-diphenylethan-2-ol)). A cationic .alpha.-olefin

polymn. catalyst was generated from this complex
 with an excess of methylaluminoxane (MeAlO)n. A comparison of the
catalytic activity with those of similar bis(alkoxide)
 complexes is presented.

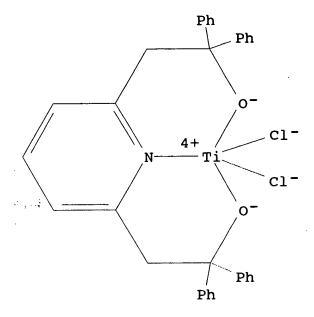
IT 203986-89-4P

(prepn. and catalytic activity in .alpha.-olefin polymn. with methylaluminoxane)

1 .

RN 203986-89-4 HCA

CN Titanium, dichloro[.alpha.,.alpha.,.alpha.',.alpha.'-tetraphenyl-2,6-pyridinediethanolato(2-)-.kappa.N1,.kappa.O2,.kappa.O6]-, (TB-5-22)-(9CI) (CA INDEX NAME)



```
78-7 (Inorganic Chemicals and Reactions)
CC
     Section cross-reference(s): 27, 67, 75
    crystal structure bisdiphenylsilyloxyethylpyridine;
ST
     silyloxydiphenylethylpyridine prepn structure reaction titanium;
     titanium pyridinebisdiphenylethanolate complex prepn
   catalyst; olefin polymn titanium
     pyridinebisdiphenylethanolato complex catalyst
    Methyl aluminoxanes
IT
        (catalytic activity in .alpha.-olefin
      polymn. with titanium pyridinebis(diphenylethanolato)
        chloro complex)
     .alpha.-Alkenes
TI
        (catalytic polymn. by titanium
        pyridinebis(diphenylethanolato) chloro complex)
     Coordination polymerization catalysts
IT
     Polymerization
        (catalytic polymn. of .alpha.-olefins
        by titanium pyridinebis(diphenylethanolato) chloro complex)
     74-85-1, Ethylene, reactions 115-07-1, Propene, reactions
ΙT
        (catalytic polymn. by titanium
        pyridinebis(diphenylethanolato) chloro complex)
     9002-88-4P, Polyethylene 9003-07-0P, Polypropylene
IT
        (catalytic polymn. of .alpha.-olefins
        by titanium pyridinebis(diphenylethanolato) chloro complex)
IT 203986-89-4P
        (prepn. and catalytic activity in .alpha.-
      ol fin polymn. with methylaluminoxane)
                         COPYRIGHT 1998 ACS
L36 ANSWER 2 OF 7 HCA
127:109005 Neutral and Cationic Zirconium Benzyl Complexes Containing
```

Bidentate Pyridine-Alkoxide Ligands. Synthesis and Ol fin Polymerization Chemistry of (pyCR20)2Zr(CH2Ph)2 and (pyCR20)2Zr(CH2Ph) + Complexes. Tsukahara, Toru; Swenson, Dale C.; Jordan, Richard F. (Department of Chemistry, University of Iowa, Iowa City, IA, 52242, USA). Organometallics, 16(15), 3303-3313 (English) 1997. CODEN: ORGND7. ISSN: 0276-7333. OTHER SOURCES: Publisher: American Chemical Society. CJACS-IMAGE; CJACS. The reaction of Zr(CH2Ph)4 with the pyridine alcs. 6-pyCR1R2OH (2a, AB R1 = R2 = CF3; 2b, R1 = R2 = Me; 2c, R1 = H, R2 = CF3) yields dibenzyl complexes (pyCR1R2O)2Zr(CH2Ph)2 (3a-c). These species adopt distorted octahedral structures with a trans-0, cis-N, cis-C ligand arrangement but undergo rapid inversion of configuration at Zr on the NMR time scale, with racemization barriers in the range from 8.6 (3b) to 10.1 (3c) kcal/mol. 3A and 3b react with B(C6F5)3 to yield [(pyCR1R2O)2Zr(CH2Ph)][PhCH2B(C6F5)3] (6a,b) and with [HNMe2Ph][B(C6F5)4] to yield [(pyCR1R20)2Zr(CH2Ph)][B(C6F5)4] (7a,b). NMR spectra indicate that 6a,b and 7a,b are not strongly ion-paired in CD2Cl2. 6A polymerizes ethylene and 1-hexene to low mol. wt. polymers. [{PyCH(CF3)O}2Zr(CH2Ph)][PhCH2B(C6F5)3] (6c, generated in situ) is much less active for ethylene polymn. than 6a, and 6b is inactive.

IT 192432-42-1P

(prepn. and thermal loss of THF from)

RN 192432-42-1 HCA

CN Zirconium, bis[.alpha.,.alpha.-bis(trifluoromethyl)-6-(trimethylsilyl)-2-pyridinemethanolato-.kappa.O2]dichlorobis(tetrahy drofuran)- (9CI) (CA INDEX NAME)

IT 192432-41-0P 192432-43-2P

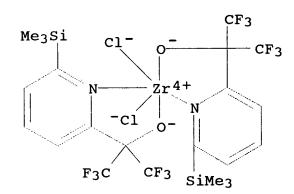
(prepn. of)

RN 192432-41-0 HCA

CN Zirconium, tris[.alpha.,.alpha.-bis(trifluoromethyl)-2pyridinemethanolato-.kappa.N1,.kappa.O2]chloro- (9CI) (CA INDEX NAME)

RN 192432-43-2 HCA

CN Zirconium, bis[.alpha.,.alpha.-bis(trifluoromethyl)-6-(trimethylsilyl)-2-pyridinemethanolato-.kappa.N1,.kappa.O2]dichloro-, (OC-6-13)- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds) Section cross-reference(s): 35, 75

olefin polymn catalyst zirconium
benzyl pyridinealkoxo; zirconium benzyl pyridinealkoxo prepn
structure catalysis; crystal structure zirconium benzyl
pyridinealkoxo complex; mol structure zirconium benzyl
pyridinealkoxo complex; racemization barrier zirconium benzyl
pyridinealkoxo

IT Polyolefins

(prepn. catalyzed by zirconium benzyl pyridinealkoxo complexes)

IT Alcohols, preparation
(pyridinealkoxides, zirconium benzyl complexes; prepn., crystal structure and catalysis of olefin polymn. by)

IT Methyl aluminoxanes

(zirconium benzyl pyridinealkoxo complex and MAO as

```
catalyst for ol fin polymn.)
    Polymerization catalysts
ΙT
        (zirconium benzyl pyridinealkoxo complexes for olefins)
IT
    50981-41-4P, Polyhexene
        (atactic; zirconium benzyl pyridinealkoxo complex as
      catalyst for prepn. of low mol. wt.)
     136040-19-2, Triphenylmethylium tetrakis(pentafluorophenyl)borate(1-
IT
    )
        (for prepn. of olefin polymn.
      catalyst from zirconium benzyl pyridinealkoxo complexes)
     1109-15-5, Tris(pentafluorophenyl)borane
IT
                                                118612-00-3,
    Dimethyl(phenyl)ammonium tetrakis(pentafluorophenyl)borate
        (for prepn. of olefin polymn.
      catalysts from zirconium benzyl pyridinealkoxo complexes)
    192432-50-1
IT
        (in situ formation and catalysis of olefin
     polymn. by)
                    192525-61-4P
IT
     192432-47-6P
        (prepn. and catalysis of olefin
     polymn.)
IT 192432-42-1P
        (prepn. and thermal loss of THF from)
     192432-37-4P 192432-41-0P 192432-43-2P
IT
                                   192432-52-3P 192525-63-6P
                    192432-51-2P
     192432-48-7P
     192525-64-7P
        (prepn. of)
ΙT
     192432-45-4
                   192525-62-5
        (prepn., fluxionality and catalysis of olefin
     polymn.)
IT
     192432-38-5P
        (prepn., soln. racemization, catalysis of
      olefin polymn. with MAO and reactions with
        triarylboron or tetraarylborate)
     9002-88-4P, Polyethylene
IT
        (zirconium benzyl pyridinealkoxo complexes as catalysts
        for prepn. of low mol. wt.)
    ANSWER 3 OF 7 HCA COPYRIGHT 1998 ACS
L36
127:75019 Synthesis, Structures, Dynamics, and Olefin
   Polymerization Behavior of Group 4 Metal (pyCAr20)2M(NR2)2
     Complexes Containing Bidentate Pyridine-Alkoxide Ancillary Ligands.
     Kim, Il; Nishihara, Yasushi; Jordan, Richard F.; Rogers, Robin D.;
     Rheingold, Arnold L.; Yap, Glenn P. A. (Department of Chemistry,
     University of Iowa, Iowa City, IA, 52242, USA). Organometallics,
     16(15), 3314-3323 (English) 1997. CODEN: ORGND7. ISSN: 0276-7333.
     OTHER SOURCES: CJACS-IMAGE; CJACS. Publisher: American Chemical
     Society.
     The reaction of 2-lithiopyridine and the appropriate diarylketone
AB
     followed by hydrolysis yields pyCAr2OH pyridine-alcs. (la, Ar =
     4-tBu-C6H4; 1b, pyCAr2OH = 2-pyridyl-9-fluorenol; 1c, Ar =
     3-CF3-C6H4; 1d, Ar = 4-Ph-C6H4; 1e, Ar = 4-NEt2-C6H4; 1f, pyCAr2OH =
```

1-(2-pyridy1)-1-dibenzosuberol; 1g, Ar = 3,5-(CF3)2-C6H3). reaction of Ti(NMe2)4 with 2 equiv of 1a-g yields (pyCAr2O)2Ti(NMe2)2 (2a-g) and NMe2H. The reaction of Zr(NMe2)4 with 2 equiv of 1a,b,e yields (pyCAr20)2Zr(NMe2)2 (3a,b,e), while similar reactions with 1c,d yield mixts. of (pyCAr20)xZr(NMe2)4-x (x ${PyC(3-CF3-C6H4)20}3Zr(NMe2)$ (4c) and = 1-3) species. {pyC(4-NEt2-C6H4)20}4Zr (5e) were prepd. from Zr(NMe2)4 and 3 equiv of 1c or 4 equiv of 1e, resp. The reaction of Hf(NMe2)4 with 2 equiv of la,e yields (pyCAr20)2Hf(NMe2)2 (6a,e), while reaction with 3 equiv of 1b,c yields (pyCAr20)3Hf(NMe2) (7b,c). X-ray crystallog. analyses establish that 2b, 2e.cntdot.toluene, and 3a.cntdot.0.5NMe2H adopt distorted octahedral structures with a trans-0, cis-py, cis-amide arrangement of ligands. NMR data show that (pyCAr2O) 2M(NMe2) 2 complexes adopt the same structure in soln. but undergo inversion of configuration at the metal with racemization barriers (.DELTA.G.thermod. (racemization)) at 12-14 kcal/mol. Treatment of (pyCAr20)2M(NMe2)2 complexes with Al(iBu)3 and methylalumoxane (MAO) yields active, multisite ethylene polymn. catalysts.

IT 191334-13-1P 191334-25-5P

(prepn. and catalyst for polymn. of ethylene)

RN 191334-13-1 HCA

CN Titanium, bis[.alpha.,.alpha.-bis([1,1'-biphenyl]-4-yl)-2pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-,
(OC-6-13)- (9CI) (CA INDEX NAME)

R

PAGE 3-A

R3
Ph

RN 191334-25-5 HCA

CN Zirconium, bis[.alpha.,.alpha.-bis[4-(diethylamino)phenyl]-2pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-,
(OC-6-13)- (9CI) (CA INDEX NAME)

PAGE 2-A



IT 191334-39-1P 191334-41-5P

(prepn. and crystal structure)

RN 191334-39-1 HCA

CN Titanium, bis[.alpha.,.alpha.-bis[4-(diethylamino)phenyl]-2pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-,
(OC-6-13)-, compd. with methylbenzene (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 191334-15-3

CMF C56 H76 N8 O2 Ti

CCI CCS

CDES 7:0C-6-13

PAGE 2-A

CM 2

CRN 108-88-3 CMF C7 H8

RN 191334-41-5 HCA

CN Zirconium, bis[.alpha.,.alpha.-bis[4-(1,1-dimethylethyl)phenyl]-2-pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-, (OC-6-13)-, compd. with N-methylmethanamine (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 191334-21-1

CMF C56 H72 N4 O2 Zr

CCI CCS

CDES 7:OC-6-13

CM 2

CRN 124-40-3 CMF C2 H7 N

 $_{\mathrm{H_3C}-\mathrm{NH}-\mathrm{CH_3}}$

IT 191334-09-5P

(prepn. and crystal structure and **catalyst** for polymn. of ethylene)

RN 191334-09-5 HCA

CN Titanium, bis(N-methylmethanaminato)bis[9-(2-pyridinyl-.kappa.N)-9H-fluoren-9-olato-.kappa.O]-, (OC-6-13)- (9CI) (CA INDEX NAME)

IT 191334-15-3P

(prepn. and mol. structure and catalyst for polymn. of ethylene)

RN 191334-15-3 HCA

CN Titanium, bis[.alpha.,.alpha.-bis[4-(diethylamino)phenyl]-2pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-,
(OC-6-13)- (9CI) (CA INDEX NAME)

PAGE 2-A



IT 191334-11-9P 191334-17-5P 191334-19-7P 191334-31-3P 191334-33-5P

(prepn. and racemization barrier)

RN 191334-11-9 HCA

Titanium, bis[.alpha.,.alpha.-bis[3-(trifluoromethyl)phenyl]-2pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-,
(OC-6-13)- (9CI) (CA INDEX NAME)

PAGE 2-A

$$Me = N$$
 Me

RN 191334-17-5 HCA
CN Titanium, bis[10,11-dihydro-5-(2-pyridinyl-.kappa.N)-5Hdibenzo[a,d]cyclohepten-5-olato-.kappa.O]bis(N-methylmethanaminato), (OC-6-13)- (9CI) (CA INDEX NAME)

RN 191334-19-7 HCA
CN Titanium, bis[.alpha.,.alpha.-bis[3,5-bis(trifluoromethyl)phenyl]-2pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-,
(OC-6-13)- (9CI) (CA INDEX NAME)

RN 191334-31-3 HCA

CN Hafnium, bis[.alpha.,.alpha.-bis[4-(1,1-dimethylethyl)phenyl]-2pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-,
(OC-6-13)- (9CI) (CA INDEX NAME)

RN 191334-33-5 HCA
CN Hafnium, bis[.alpha.,.alpha.-bis[4-(diethylamino)phenyl]-2pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-,
(OC-6-13)- (9CI) (CA INDEX NAME)

IT 191334-23-3P 191334-27-7P 191334-35-7P 191334-37-9P

(prepn. of)

RN 191334-23-3 HCA

CN Zirconium, bis(N-methylmethanaminato)bis[9-(2-pyridinyl-.kappa.N)-9H-fluoren-9-olato-.kappa.O]-, (OC-6-13)- (9CI) (CA INDEX NAME)

RN 191334-27-7 HCA

CN Zirconium, bis[.alpha.,.alpha.-bis[3-(trifluoromethyl)phenyl]-2-pyridinemethanolato-.kappa.N1,.kappa.O2][.alpha.,.alpha.-bis[3-(trifluoromethyl)phenyl]-2-pyridinemethanolato-.kappa.O2](N-methylmethanaminato)- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 191334-35-7 HCA

CN Hafnium, (N-methylmethanaminato)bis[9-(2-pyridinyl-.kappa.N)-9H-fluoren-9-olato-.kappa.O][9-(2-pyridinyl)-9H-fluoren-9-olato-.kappa.O]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 191334-37-9 HCA

CN Hafnium, bis[.alpha.,.alpha.-bis[3-(trifluoromethyl)phenyl]-2pyridinemethanolato-.kappa.N1,.kappa.O2][.alpha.,.alpha.-bis[3(trifluoromethyl)phenyl]-2-pyridinemethanolato-.kappa.O2](Nmethylmethanaminato)- (9CI) (CA INDEX NAME)

IT 191334-07-3P

(prepn., racemization barrier and catalyst for polymn. of ethylene)

RN 191334-07-3 HCA

CN Titanium, bis[.alpha.,.alpha.-bis[4-(1,1-dimethylethyl)phenyl]-2-pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-, (OC-6-13)- (9CI) (CA INDEX NAME)

PAGE 2-A

(prepn., racemization barrier, mol. structure and catalyst for polymn. of ethylene)

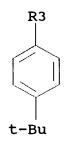
191334-21-1 HCA

RN

CN

Zirconium, bis[.alpha.,.alpha.-bis[4-(1,1-dimethylethyl)phenyl]-2-pyridinemethanolato-.kappa.N1,.kappa.O2]bis(N-methylmethanaminato)-, (OC-6-13)- (9CI) (CA INDEX NAME)

PAGE 2-A



78-7 (Inorganic Chemicals and Reactions) CC

Section cross-reference(s): 23, 27, 35, 67, 75 crystal structure titanium zirconium pyridinemethanolato amido; STGroup 4 pyridinemethanolato amido prepn structure; titanium pyridinemethanolato amido catalyst prepn structure; zirconium pyridinemethanolato amido catalyst prepn structure; olefin polymn catalyst

titanium zirconium pyridinemethanolato; ethylene polymn catalyst titanium zirconium pyridinemethanolato

Polymerization catalysts IT

4 ()

(catalytic polymn. of ethylene by titanium and zirconium and hafnium pyridinemethanolato dimethylamido complexes)

Group IVB element complexes IT

(prepn., crystal structure and racemization in soln. of Group 4 pyridinemethanolato dimethylamido complex olefin polymn. catalysts)

74-85-1, Ethene, reactions 9002-88-4, Polyethylene ΙT (catalytic polymn. of ethylene by titanium and zirconium and hafnium pyridinemethanolato dimethylamido complexes)

TI3275-24-9, Tetrakis(dimethylamido)titanium 19756-04-8, Tetrakis (dimethylamido) zirconium 19782-68-4, Tetrakis (dimethylamido) hafnium

(for prepn. of Group 4 pyridinemethanolato dimethylamido complex catalyst for ethylene polymn.)

149064-67-5, Bis(4-tert-butylphenyl)-2-pyridylmethanol ΙT (for prepn. of Group 4 pyridinemethanolato dimethylamido complex olefin polymn. catalysts)

64436-62-0P, 9-(2-Pyridyl)-9-fluorenol 95425-83-5P, IT 1-(2-Pyridyl) dibenzosuberol 191333-98-9P, Bis(3ي د خه ه

```
(trifluoromethyl)phenyl)-2-pyridylmethanol
                                                  191334-00-6P
     191334-02-8P, Bis(4-(diethylamino)phenyl)-2-pyridylmethanol
     191334-05-1P, Bis(3,5-bis(trifluoromethyl)phenyl)-2-pyridylmethanol
        (for prepn. of Group 4 pyridinemethanolato dimethylamido complex
     olefin polymn. catalysts)
     90-93-7, 4,4'-Bis(diethylamino)benzophenone
                                                   109-04-6,
IT
                       486-25-9, 9-Fluorenone
                                                1210-35-1,
     2-Bromopyridine
                       1868-00-4, 3,3'-Bis(trifluoromethyl)benzophenone
    Dibenzosuberone
     3478-90-8, 4,4'-Diphenylbenzophenone
                                            175136-66-0,
     3,3',5,5'-Tetrakis(trifluoromethyl)benzophenone
        (for prepn. of pyridinemethanol aryl deriv. and its Group 4
        pyridinemethanolato dimethylamido complex catalyst for
        ethylene polymn.)
IT 191334-13-1P 191334-25-5P
        (prepn. and catalyst for polymn. of ethylene)
IT 191334-39-1P 191334-41-5P
        (prepn. and crystal structure)
IT 191334-09-5P
        (prepn. and crystal structure and catalyst for polymn.
        of ethylene)
IT 191334-15-3P
        (prepn. and mol. structure and catalyst for polymn. of
        ethylene)
IT 191334-11-9P 191334-17-5P 191334-19-7P
   191334-31-3P 191334-33-5P
        (prepn. and racemization barrier)
IT 191334-23-3P 191334-27-7P
                             191334-29-9P
   191334-35-7P 191334-37-9P
        (prepn. of)
IT 191334-07-3P
        (prepn., racemization barrier and catalyst for polymn.
        of ethylene)
IT 191334-21-1P
        (prepn., racemization barrier, mol. structure and
      catalyst for polymn. of ethylene)
    ANSWER 4 OF 7 HCA COPYRIGHT 1998 ACS
126:277883 Olefin polymerization catalyst
     component, catalyst containing it, and use of the
   catalyst to produce olefin polymers.
     Katayama, Hiroaki; Nabika, Masaaki; Imai, Akio; Kawamura, Norio;
     Hanaoka, Hidenori (Sumitomo Chemical Company, Limited, Japan). Eur.
     Pat. Appl. EP 761694 A1 970312, 23 pp. DESIGNATED STATES: R: BE,
                          (English). CODEN: EPXXDW. APPLICATION: EP
     DE, FR, GB, IT, NL.
     96-305908 960812. PRIORITY: JP 95-205953 950811.
GΙ
```

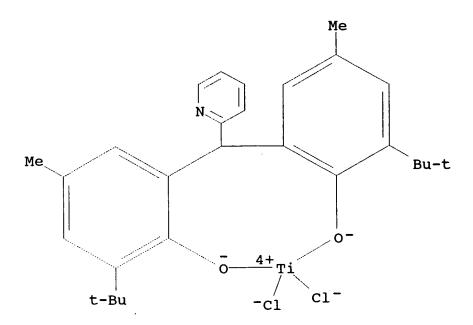
The component is represented by the general formula I, in which A AB and A1 are C1-50 (halogenated) hydrocarbylene optionally bearing an O-contg. substituent, M is a Group 4 transition metal or a lanthanide, Q is a trivalent residue contg. a Group 13-15 element, X and X1 are halogen or C1-20 hydrocarbyl, and Y is a C1-20 (halogenated) hydrocarbon group contg. .gtoreq.1 hetero atom. Catalyst systems contg. I are highly active at advantageous polymn. temps., give polyolefins of high mol. wt., and require a reduced amt. of organoaluminum cocatalyst. 2-tert-butyl-4-methylphenol was treated with MeMgBr, condensed with 2-thiophenecarboxaldehyde, and hydrolyzed to give the bisphenol, which reacted with TiCl4 to give orange solid II. Copolymn. of ethylene with 1-hexene in toluene at 80.degree. in the presence of Et3Al 250, II 5.0, and Ph3C+ -B(C6F5)4 15 .mu.mol gave a copolymer with wt.-av. mol. wt. 1.7 .times. 105, mol.-wt. distribution 2.6, and 19.8 short-chain branches per 1000 chain C atoms at a catalyst yield of 1.7 .times. 106 g copolymer per mol Ti.

IT 188841-53-4P

(prepn. of **olefin polymn. catalyst** component)

RN 188841-53-4 HCA

CN Titanium, dichloro[[2,2'-(2-pyridinylmethylene)bis[6-(1,1-dimethylethyl)-4-methylphenolato-.kappa.O]](2-)]-, (T-4)- (9CI) (CA INDEX NAME)



component)

184864-66-2P

184864-78-6P

184864-52-6P

184864-75-3P

IT

```
C08F004-642
IC
     ICM
     ICS C08F010-02; C07F007-00
     35-3 (Chemistry of Synthetic High Polymers)
CC
     olefin polymn catalyst component;
ST
     bisphenol dichlorotitanate catalyst
     Linear low-density polyethylenes
IT
        (olefin polymn. catalyst component
        for manuf. of)
IT
     Aluminoxanes
        (olefin polymn. catalyst component
        for use with)
IT
     Polymerization catalysts
        (prepn. of olefin polymn. catalyst
        component)
IT
     25213-02-9P, Ethylene-1-hexene copolymer
        (olefin polymn. catalyst component
        for manuf. of)
                                        100-99-2, Triisobutylaluminum,
     97-93-8, Triethylaluminum, uses
IT
            136040-19-2, Triphenylmethyl tetrakis(pentafluorophenyl)borat
     uses
        (olefin polymn. catalyst component
        for use with)
                                                 188841-56-7P
                                  188841-54-5P
IT
     188841-52-3P 188841-53-4P
                                                    188841-61-4P
                                    188841-59-0P
     188841-57-8P
                    188841-58-9P
                    188841-63-6P
                                    188841-65-8P
     188841-62-5P
        (prepn. of ol fin polymn. catalyst
```

184864-69-5P

184864-84-4P

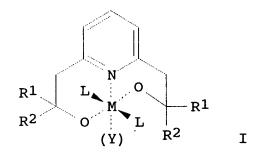
184864-72-0P

185151-28-4P

188841-55-6P 188841-60-3P 188841-64-7P (prepn. of ol fin polymn. catalyst component)

98-03-3, 2-Thiophenecarboxaldehyde 105-67-9, 2,4-Xylenol IT 106-44-5, p-Cresol, reactions 121-00-6, 2-tert-Butyl-4methoxyphenol 497-39-2 1121-60-4, Picolinaldehyde 3541-37-5, 2-2-tert-Butyl-4-methylphenol 10323-39-4, 4-Bromo-2-tert-Benzothiophenecarboxaldehyde 13679-70-4, 5-Methyl-2-thiophenecarboxaldehyde butylphenol 19909-85-4, Dichloro(4-methoxyphenyl)phosphine 26421-44-3, 2,5-Dimethyl-3-thiophenecarboxaldehyde (prepn. of olefin polymn. catalyst component)

L36 ANSWER 5 OF 7 HCA COPYRIGHT 1998 ACS
126:225669 Pyridine-containing transition metal complexes as
olefin polymerization catalysts. Igai,
Shigeru; Imaoka, Koji; Mitani, Nobuhiro (Ube Industries, Japan).
Jpn. Kokai Tokkyo Koho JP 09012582 A2 970114 Heisei, 8 pp.
(Japanese). CODEN: JKXXAF. APPLICATION: JP 95-165160 950630.



1. 1. 2. 4

The catalysts comprise I (R1, R2 = H, hydrocarbyl; R1R2 may form a bridged ring; L = H, halo, hydrocarbyl; M = Group IV metal; Y = heteroatom-contg. electron donor; m = 0, 1, 2; n = 1, 2), and organoaluminum oxy compds. and/or B-contg. ionic compds. Thus, ethylene was polymd. in the presence of I (R1R2 = 2-adamantyl, L = C1, M = Zr, Y = THF) 5, Ph3C+.cntdot.(BPh4) - 5, and triisobutylaluminum 300 .mu.M in PhMe at 40.degree. to give polymers with Mw 1,320,000, and Mw/Mn 2.7. The catalyst activity was 89.4 g/mmol-Zr/h.

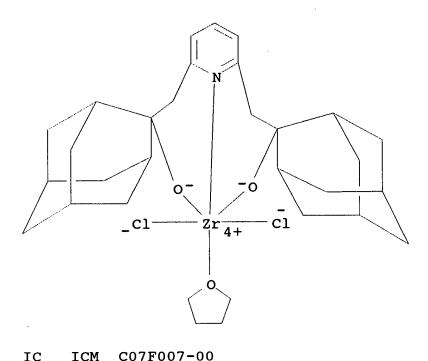
IT 188032-56-6P

(pyridine-contg. transition metal complexes as **olefin polymn. catalysts**)

RN 188032-56-6 HCA

CN Zirconium, dichloro[[2,2'-[(2,6-pyridinediyl-

- .kappa.N)bis(methylene)]bis[tricyclo[3.3.1.13,7]decan-2-olato-
- .kappa.O]](2-)](tetrahydrofuran)- (9CI) (CA INDEX NAME)



IC

IT

21959-01-3

```
C07F007-00; C07F007-28; C08F004-76; C08F010-00
     ICS
     35-3 (Chemistry of Synthetic High Polymers)
CC
     Section cross-reference(s): 27, 67
     pyridine transition metal complex catalyst; olefin
ST
     pyridine zirconium complex polymn catalyst;
     adamantyl pyridine zirconium complex polymn catalyst;
     ethylene pyridine zirconium complex polymn catalyst
IT
     Polymerization catalysts
        (pyridine-contg. transition metal complexes as olefin
      polymn. catalysts)
     Methyl aluminoxanes
IT
        (pyridine-contg. transition metal complexes as olefin
      polymn. catalysts)
     Polyolefins
IT
        (pyridine-contg. transition metal complexes as olefin
      polymn. catalysts)
     100-99-2, Triisobutylaluminum, uses
                                           117802-41-2, Trityl
IT
     tetraphenylborate
        (pyridine-contg. transition metal complexes as olefin
      polymn. catalysts)
IT 188032-56-6P
        (pyridine-contg. transition metal complexes as olefin
      polymn. catalysts)
     9002-88-4P, Polyethylene
IT
        (pyridine-contg. transition metal complexes as olefin
      polymn. catalysts)
```

149903-53-7

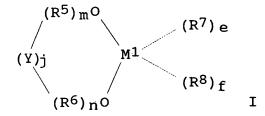
(pyridine-contg. transition metal complexes as **olefin** polymn. catalysts)

L36 ANSWER 6 OF 7 HCA COPYRIGHT 1998 ACS 122:106775 Catalysts for polymerization of

olefins and manufacture of olefin

copolymers. Yokota, Kiyohiko; Tani, Noriyuki; Watanabe, Masami; Kawasaki, Nobuo (Idemitsu Kosan Co, Japan). Jpn. Kokai Tokkyo Koho JP 06192330 A2 940712 Heisei, 14 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 93-257671 930921. PRIORITY: JP 92-279372 920924.

GΙ



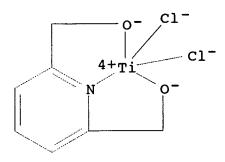
Olefin copolymers are manufd. with catalysts comprising transition metal compds. I [M1 = Group 3-10 or lanthanide metal; R5, R6 = C1-20 hydrocarbylene; R7, R8 = .sigma.-bonding ligand, chelating ligand, Lewis base; Y = C1-20 hydrocarbylene, XR9R10, O, S; R9, R10 = C1-20 hydrocarbyl; X = C, N, S, P, Si; e, f = 0-2; e + f = (valence of M1) - 2; j = 0-4; m, n = 0, 1], ionic compds. forming complexes with I, and optional organoaluminum compds. Thus, 40 mL 1-octene was copolymd. with ethylene at 80.degree. and 8 atm in PhMe in a 1-L autoclave in the presence of iso-Bu3A1, [2,2'-thiobis(6-tert-butyl-4-methylphenoxy)]titanium dichloride, and PhNMe2HB(C6F5)4 for 1 h to give 0.60 g copolymer showing intrinsic viscosity 9.25 dL/g and m.p. 79.degree.

IT 160758-51-0 160758-52-1

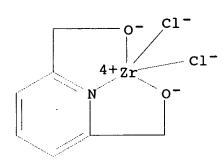
(transition metal-ionic compd. catalysts for polymn. of olefins)

RN 160758-51-0 HCA

CN Titanium, dichloro[2,6-pyridinedimethanolato(2-)-N1,0.alpha.,0.alpha.']-(9CI) (CA INDEX NAME)



RN 160758-52-1 HCA
CN Zirconium, dichloro[2,6-pyridinedimethanolato(2-)N1,0.alpha.,0.alpha.']- (9CI) (CA INDEX NAME)



polymn. of ol fins)

IC ICM C08F010-00 C08F004-642 35-3 (Chemistry of Synthetic High Polymers) CC STolefin polymn catalyst transition metal; complex transition metal catalyst polymn IT Polymerization catalysts (transition metal-ionic compd. catalysts for polymn. of olefins) IT Alkenes, preparation (polymers, transition metal-ionic compd. catalysts for polymn. of olefins) ΙT 100-99-2, Triisobutylaluminum, uses 1109-15-5, 13523-46-1 104901-00-0 Tris(pentafluorophenyl)boron 111215-59-9, 2,2'-Thiobis(6-tert-butyl-4-104901-01-1 110301-92-3 methylphenoxy)titanium dichloride 118612-00-3 159804-08-7, Dibenzyl[2,2'-thiobis(6-tert-butyl-4-methylphenoxy)]titanium 160481-72-1 **160758-51-0 160758-52-1** 160758-53-2 160758-54-3 (transition metal-ionic compd. catalysts for polymn. of ol fins) IT26221-73-8P 9002-88-4P (transition metal-ionic compd. catalysts for

L36 ANSWER 7 OF 7 HCA COPYRIGHT 1998 ACS

121:280477 Polymer-immobilized manganese(III)-Schiff base complexes for catalytic epoxidation of olefins. Fujii, Yuki; Ebina, Fujio; Yanagisawa, Manabu; Matsuoka, Hitoshi; Kato, Tohru (Fac. Sci., Ibaraki Univ., Ibaraki, 310, Japan). J. Inorg. Organomet. Polym., 4(3), 273-88 (English) 1994. CODEN: JIOPE4. ISSN:

1053-0495. OTHER SOURCES: CASREACT 121:280477.

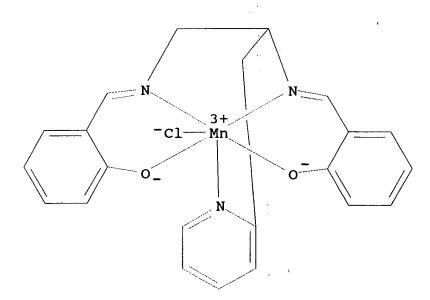
Polymer-linked manganese(III)-salen-type Schiff base complexes were prepd. by the copolymn. of functionalized Schiff base, styrene, and divinylbenzene at various mixing ratios (1:10:0-1:12:4), followed by introduction of Mn(III) ion. The materials catalyzed epoxidn. of cyclohexene with iodosylbenzene in CH2Cl2 as rapidly as the monomer complexes. The max. total turnover reached 170, which is about 13 times higher than that of the monomer. The lifetime of polymer catalysts is discussed in terms of crosslinking and solvent effects.

IT 158989-20-9

(prepn. of polymer-immobilized manganese-Schiff base complexes for **catalytic** epoxidn. of olefins)

RN 158989-20-9 HCA

CN Manganese, chloro[[2,2'-[[1-(2-pyridinylmethyl)-1,2-ethanediyl]bis(nitrilomethylidyne)]bis[phenolato]](2-)-N,N',N'',O,O']-, (OC-6-65)- (9CI) (CA INDEX NAME)



- CC 27-2 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 67, 78
- ST polymer immobilized manganese Schiff base complex; epoxidn catalyst olefin polymer immobilized manganese
- IT Alkenes, reactions

```
(catalytic epoxidn. of)
    Epoxidation catalysts
IT
    Polymer-supported reagents
    Solvent effect
        (prepn. of polymer-immobilized manganese-Schiff base complexes
        for catalytic epoxidn. of olefins)
                  53177-12-1
                               73808-82-9
                                            80778-81-0
                                                         158989-19-6
IT
     27658-88-4
                               158989-22-1
                 158989-21-0
   158989-20-9
        (prepn. of polymer-immobilized manganese-Schiff base complexes
        for catalytic epoxidn. of olefins)
     7439-96-5DP, Manganese, polymer supported salen and styrene
IT
    divinylbenzene complexes 27658-88-4DP, styrene divinylbenzene
                         53177-12-1DP, styrene divinylbenzene polymer
    polymer supported
                 158959-83-2DP, manganese chloride complexes
     158959-84-3DP, manganese chloride complexes
                                                   158959-85-4DP,
                                    158959-86-5DP, manganese chloride
    manganese chloride complexes
     complexes
        (prepn. of polymer-immobilized manganese-Schiff base complexes
        for catalytic epoxidn. of olefins)
     90-02-8, Salicylaldehyde, reactions
                                           107-15-3, 1,2-Ethanediamine,
IT
                 110-83-8, Cyclohexene, reactions
     reactions
                                                    536-80-1,
                                   158959-80-9
                      58813-73-3
                                                 158959-82-1
     Iodosylbenzene
        (prepn. of polymer-immobilized manganese-Schiff base complexes
        for catalytic epoxidn. of olefins)
                                                  158959-85-4P
                                   158959-84-3P
                    158959-83-2P
IT
     158959-81-0P
     158959-86-5P
        (prepn. of polymer-immobilized manganese-Schiff base complexes
        for catalytic epoxidn. of olefins)
=> d his 138-
     (FILE 'REGISTRY' ENTERED AT 14:16:32 ON 04 AUG 1998)
     FILE 'HCA' ENTERED AT 14:17:22 ON 04 AUG 1998
             48 S L37 NOT 1995-1997/PY
L38
=> d 138 1-48 cbib abs hitstr hitind
    ANSWER 1 OF 48 HCA COPYRIGHT 1998 ACS
123:73254 New mixed complexes of Zr (IV) with mono and multidentate
              Tarafder, M. T. H.; Islam, M. Shamsul; Bhattacharjee, P.;
     Quraishi, S. B. (Department of Chemistry, Rajshahi University,
     Rajshahi, Bangladesh). Pak. J. Sci. Ind. Res., 37(4), 126-8
     (English) 1994. CODEN: PSIRAA.
                                      ISSN: 0030-9885.
     Several new complexes of Zr (IV) contg. a no. of monodentate and
AB
     multidentate org. ligands were synthesized and characterized. The
     complexes have the compns., [Zr(0)Cl2(en).H2O], [Zr(0)Cl2.2L.H2O],
```

[Zr.L'3Cl] and [Zr(0)Cl2.L''] [en = ethylenediamine; L = OPPh3,

o-aminophenol, L'' = diethylenetriamine and triethylenetetramine]. The molar conductance data indicate that complexes [Zr(C9H6NO)3Cl]

OAsPh3, pyridine or aniline; HL' = 8-hydroxoquinoline,

and [Zr(C6H4NH2O)3Cl] are 1:1 electrolytes but all other complexes behave as 2:1 electrolytes. The exptl. data are consistent with 6-fold coordination of Zr (IV) ion in all the complexes excepting [Zr(C9H6NO)3Cl] [Zr(C6H4NH2O)3Cl] and [Zr(O)Cl2.tet] which are seven coordinated.

IT 165182-50-3P

(prepn. of)

RN 165182-50-3 HCA

CN Zirconium, chlorotris(8-quinolinolato-N1,08) - (9CI) (CA INDEX NAME)

CC 78-7 (Inorganic Chemicals and Reactions)
IT 165182-45-6P 165182-46-7P 165182-47-8P 165182-48-9P
165182-49-0P 165182-50-3P 165182-51-4P 165182-52-5P
165182-53-6P
(prepn. of)

L38 ANSWER 2 OF 48 HCA COPYRIGHT 1998 ACS
120:270657 Dissociation of zirconocene hydridochloride. Zhang, YunWen;
Bai, LingJun; Xu, YuMing; Li, JiangSheng; Wang, JiTao (Dep. Chem.,
Nankai Univ., Tianjin, 300071, Peop. Rep. China). Prog. Nat. Sci.,
3(1), 83-8 (English) 1993. CODEN: PNASEA. OTHER SOURCES: CASREACT
120:270657.

GI

Ι

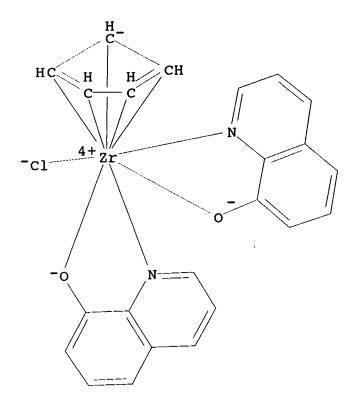
Dissocn. of zirconocene hydridochloride, CpZrHCl, was examd. by substitution reaction with phosphorus and nitrogen ligands, L, under thermal or photolytic conditions to give Zr(III) as Cp2ZrClL complex stable for several weeks without oxygen. Cp2ZrClL decomps. in air to give (Cp2ZrCl)2O and L. It was concluded that Zr-H bond experiences homolytic reaction under heating and irradn. without active hydrogen. The heterolytic reaction of Cp2ZrClH with nitrogen-contg. hydroxyl compds. was shown to give Zr-contg. heterocyclic organometallics, e.g., I. I was characterized by x-ray crystallog.

IT 12114-15-7P

(prepn. and crystal and mol. structure of)

RN 12114-15-7 HCA

CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(8-quinolinolato-N1,08)-, stereoisomer (9CI) (CA INDEX NAME)



IT 148484-15-5P 148484-16-6P 154426-19-4P

(prepn. of) 148484-15-5 HCA

RN

Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(5,7-dibromo-8-quinolinolato-N1,08)-, stereoisomer (9CI) (CA INDEX NAME) CN

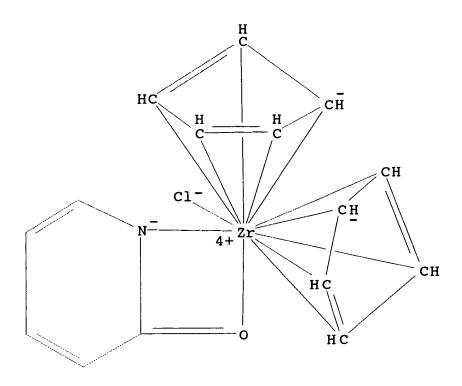
PAGE 1-A

PAGE 2-A

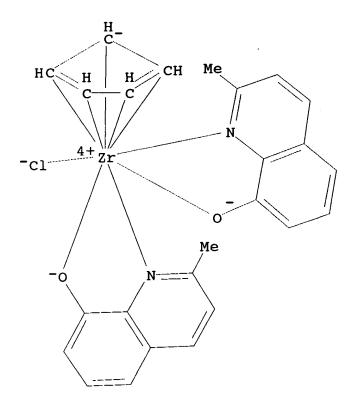
\ Br

RN 148484-16-6 HCA

CN Zirconium, chlorobis(.eta.5-2,4-cyclopentadien-1-yl)(2(1H)-pyridinonato-N1,02)- (9CI) (CA INDEX NAME)



RN 154426-19-4 HCA CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(2-methyl-8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)



29-10 (Organometallic and Organometalloidal Compounds) CC Section cross-reference(s): 75 IT 12114-15-7P

(prepn. and crystal and mol. structure of)

12097-04-0P 148484-15-5P 148484-16-6P IT

148484-17-7P 154426-19-4P

(prepn. of)

ANSWER 3 OF 48 HCA COPYRIGHT 1998 ACS

119:84507 Heterobimetallic platinum-titanium complexes: potential anticancer drugs. Berardini, M.; Emge, T. J.; Brennan, J. G. (Dep. Chem., Rutgers Univ., Piscataway, NJ, 08855-0939, USA). Inorg. Chem., 32(12), 2724-8 (English) 1993. CODEN: INOCAJ. 0020-1669. OTHER SOURCES: CJACS-IMAGE; CJACS.

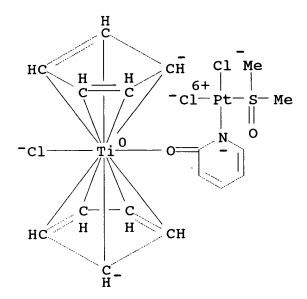
Heterobimetallic complexes contg. titanocene chloride and AB trans-PtCl2(DMSO) functional groups were prepd. by bridging the metal centers with hydroxypyridine (HL), to explore the possibility that a chelate effect will enhance DNA-metal binding affinity and chemotherapeutic effectiveness. The structure of trans-PtCl2(DMSO)(L-2-Ti(C5H5)2Cl) was detd.: monoclinic, space group Cc, a 6.958(2), b 18.047(3), c 33.217(5) .ANG., .beta. 92.04(2).degree., Z = 4, R = 0.049, Rw = 0.067. Both metal coordination environments are virtually identical to related monometallic complexes.

IT 149063-33-2P

(prepn. and crystal structure and potential anticancer activity of)

RN 149063-33-2 HCA

CN Titanium, chlorobis(.eta.5-2,4-cyclopentadien-1-yl)[dichloro[sulfinylbis[methane]-S]platinum][.mu.-(2(1H)-pyridinonato-N1:O2)]-, stereoisomer (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 1, 29, 75

IT 149063-33-2P

(prepn. and crystal structure and potential anticancer activity of)

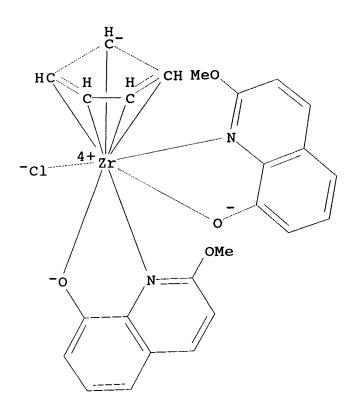
ANSWER 4 OF 48 HCA COPYRIGHT 1998 ACS 119:49507 Syntheses and characterization of heterocyclic compounds of zirconium(IV). Wang, Jitao; Zhang, Yunwen; Xiu, Yuming; Li, Jiangsheng; Gong, Yousheng (Dep. Chem., Nankai Univ., Tianjin, 300071, Peop. Rep. China). Chem. Res. Chin. Univ., 8(3), 212-18 (English) 1992. CODEN: CRCUED. OTHER SOURCES: CASREACT 119:49507. The Zr-H bond of zirconocene hydridochloride was heterolyzed at room AB temp. by 5 compds. contg. nitrogen and an hydroxyl group to give Cp(Q)2ZrCl (I, QH = 8-quinolinol, 2-methoxy-8-quinolinol, 5,7-dibromo-8-quinolinol, 2-pyridol, ethanolamine) which were characterized by elemental anal., IR, and 1H NMR spectroscopy. mol. structure of I (QH = 8-quinolinol) was confirmed by x-ray diffraction detn. The coordination polyhedron around the Zr atom can be described as a distorted octahedron. The Zr-N bonds of 0.2364(3) and 0.2377(4) nm suggest that they are coordination bonds. The two planar 8-quinolinoyl groups act as bidentate ligands chelated with Zr, forming a dihedral angle of 108.4(1).degree..

IT 148484-14-4P 148484-15-5P 148484-16-6P

(prepn. and fluorescence of)

RN 148484-14-4 HCA

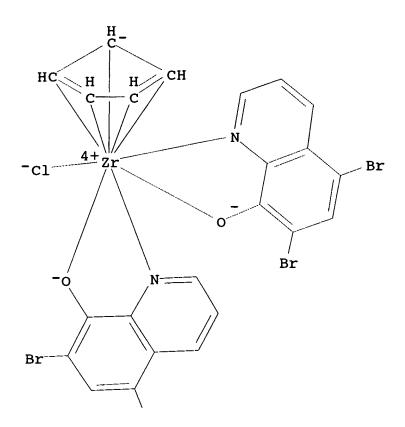
CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(2-methoxy-8-quinolinolato-N1,O8)-, stereoisomer (9CI) (CA INDEX NAME)



RN 148484-15-5 HCA

CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(5,7-dibromo-8-quinolinolato-N1,08)-, stereoisomer (9CI) (CA INDEX NAME)

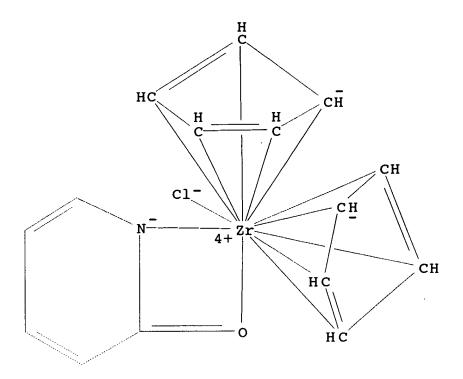
PAGE 1-A



PAGE 2-A

в̀т

RN 148484-16-6 HCA CN Zirconium, chlorobis(.eta.5-2,4-cyclopentadien-1-yl)(2(1H)-pyridinonato-N1,O2)- (9CI) (CA INDEX NAME)

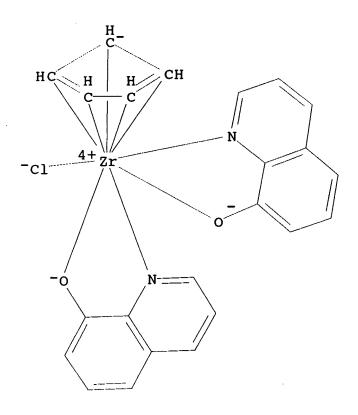


IT 12114-15-7P

(prepn., crystal structure, and fluorescence of)

RN 12114-15-7 HCA

CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(8-quinolinolato-N1,08)-, stereoisomer (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds) Section cross-reference(s): 75

IT 148484-14-4P 148484-15-5P 148484-16-6P

148484-17-7P

(prepn. and fluorescence of)

IT 12114-15-7P

(prepn., crystal structure, and fluorescence of)

L38 ANSWER 5 OF 48 HCA COPYRIGHT 1998 ACS
116:21104 Hydrosilylation of titanates containing allyl aromatic radicals. Suvorov, A. L.; Khonina, T. G.; Kodess, M. I.; Podol'skii, A. V. (Inst. Khim., Sverdlovsk, USSR). Zh. Obshch. Khim., 61(6), 1383-9 (Russian) 1991. CODEN: ZOKHA4. ISSN: 0044-460X.

GI

AB The hydrosilylation reactivity of titanates I (R=R2=Me, R1=allyl; R=R1=H, R2=allyl) by MeSiHR32 (R3=Ph, CH2Ph, C5H11) was governed by steric effects, and the extent of hydrosilylation depended on the extent of allyl-propenyl isomerization.

IT 138142-58-2

(hydrosilylation of)

RN 138142-58-2 HCA

CN Titanium, dibutoxybis[7-(2-propenyl)-8-quinolinolato-0]-, (T-4)-(9CI) (CA INDEX NAME)

CC 29-6 (Organometallic and Organometalloidal Compounds)
IT 16709-91-4, Dibenzylmethylvinylsilane 18042-43-8 132410-71-0
138142-57-1 138142-58-2 138142-59-3 138166-09-3
(hydrosilylation of)

L38 ANSWER 6 OF 48 HCA COPYRIGHT 1998 ACS

109:129860 Manufacture of titanoxane-siloxanes from silicic acid and titanium alkoxides. Misono, Takahisa; Abe, Yoshisaki; Hikita, Michiro; Nagao, Yukinori (Nissan Chemical Industries, Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 63056530 A2 880311 Showa, 5 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 86-200877 860827.

GΙ

Titanoxane-siloxanes, non-gel solids at ambient temps., stable, and convertible by hydrolytic or thermal polycondensation into inorg. polymers, are prepd. by refluxing bis(8-oxyquinolinato)titanium dialkoxides I (R = C1-4 alkyl) or (R2COCH:CR10)2Ti(OR)2 (II; R1 = C1-3 alkyl, Ph; R2 = C1-3 alkyl, C1-3 alkoxy, Ph, OPh, OCH2Ph; R1 and R2 are not Me simultaneously) with silicic acid at mol ratio SiO2/TiO2 0.25-4 in a solvent. A THF soln. (11.8 parts) of silicic acid (0.6 part SiO2) and 30 parts Me2CO soln. of 3.9 parts II (R = Bu, R1 = Me, R2 = OEt) were mixed and refluxed for 30 min to give 4.3 parts polymer which showed mol ratio SiO2/TiO2 1, and which was pulled into a 110-cm-long thread by a glass rod, and did not gel and retained its threading property when left in air for 120 h.

IT 23329-68-2

(polycondensation of, with silicic acid, titanoxane-siloxanes from)

RN 23329-68-2 HCA

CN Titanium, diethoxybis(8-quinolinolato-N1,O2)- (9CI) (CA INDEX NAME)

IC ICM C08G077-58

CC 35-4 (Chemistry of Synthetic High Polymers)

IT 20753-28-0 23329-68-2 116075-48-0, Bis(ethyl-3-phenyl-3-oxopropanoate)titanium diisopropoxide

(polycondensation of, with silicic acid, titanoxane-siloxanes from)

L38 ANSWER 7 OF 48 HCA COPYRIGHT 1998 ACS

105:202079 Composition and stability of niobium(V), zirconium(IV), yttrium(III) and lanthanum(III) chelates with 7-nitroso-8-quinolinone-5-sulfonate. El-Haty, M. T.; Adam, F. A. (Chem. Dep., Fac. Sci., Aswan, Egypt). Bull. Soc. Chim. Fr. (3), 351-4 (English) 1986. CODEN: BSCFAS. ISSN: 0037-8968.

AB New Nb(V), Zr(IV), Y(III) and La(III) chelates obtained from disodium 7-nitroso-8-quinolinone-5-sulfonate were studied by spectrophotometric, conductimetric and potentiometric methods. The solid chelates were prepd. and their IR spectra and elemental anal. were discussed. The ligand is bonded to the metal ion through the O atoms of nitroso and hydroxy groups. The apparent stability consts. of the complexes formed in soln. were also detd. spectrophotometrically and potentiometrically.

IT 105194-69-2P 105212-59-7P

(prepn. and IR spectrum of)

RN 105194-69-2 HCA

CN Zirconium(1+), diaquachloro[8-hydroxy-7-nitroso-5-quinolinesulfonato(2-)-07,08]-, chloride (9CI) (CA INDEX NAME)

• c1-

RN 105212-59-7 HCA

CN Zirconate(1-), diaquachlorobis[8-hydroxy-7-nitroso-5-quinolinesulfonato(2-)-07,08]-, sodium (9CI) (CA INDEX NAME)

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 68

IT 105177-47-7P 105177-48-8P 105177-50-2P 105177-51-3P
105194-68-1P 105194-69-2P 105194-70-5P
105212-59-7P
(prepn. and IR spectrum of)

L38 ANSWER 8 OF 48 HCA COPYRIGHT 1998 ACS

103:160633 Synthesis and characterization of .eta.5-cyclopentadienyl chloro zirconium(IV) complexes of 8-hydroxyquinoline N-oxide.

Sharma, S.; Sharma, A.; Goyal, K. C.; Kaushik, N. K. (Dep. Chem., Univ. Delhi, Delhi, India). Bull. Soc. Chim. Fr. (11-12, Pt. 1), 327-8 (English) 1984. CODEN: BSCFAS. ISSN: 0037-8968.

AB (.eta.5-C5H5)Zr(L)2Cl (LH = 8-hydroxyquinoline N-oxide, 5-nitro-,

AB (.eta.5-C5H5)Zr(L)2Cl (LH = 8-hydroxyquinoline N-oxide, 5-nitro-, 5,7-dinitro-, 5,7-dibromo- or 5-phenylazo-8-quinoline N-oxides) were synthesized in non-aq. medium by the reaction (.eta.5-C5H5)2ZrCl2 with 8-hydroxyquinoline N-oxide and its substituted derivs. The N-oxides behave as unineg. bidentate ligands and Zr is hexacoordinate in all the complexes.

IT 98606-19-0P 98606-20-3P 98606-21-4P 98606-22-5P 98606-31-6P

(prepn. and spectra of)

RN 98606-19-0 HCA

CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(5,7-dibromo-8-quinolinol 1-oxidato-0,0')- (9CI) (CA INDEX NAME)

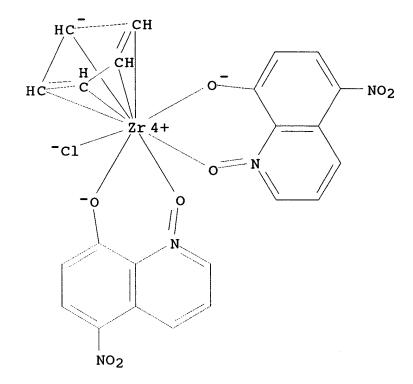
RN 98606-20-3 HCA

CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis[5-(phenylazo)-8-quinolinol 1-oxidato-0,0']- (9CI) (CA INDEX NAME)

RN 98606-21-4 HCA CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)(8-quinolinol 1-oxidato-0,0')- (9CI) (CA INDEX NAME)

RN 98606-22-5 HCA

CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(5-nitro-8-quinolinol 1-oxidato-01,08)- (9CI) (CA INDEX NAME)



RN 98606-31-6 HCA

CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(5,7-dinitro-8-quinolinol 1-oxidato-01,08)- (9CI) (CA INDEX NAME)

CC 29-10 (Organometallic and Organometalloidal Compounds)
IT 98606-19-0P 98606-20-3P 98606-21-4P
98606-22-5P 98606-31-6P
(prepn. and spectra of)

L38 ANSWER 9 OF 48 HCA COPYRIGHT 1998 ACS

102:105073 Chelated titanium(IV) derivatives of 1,1-diphenylethanol and phenolphthalein. Deshpande, S. S.; Awasarkar, P. A.; Gopinathan, Sarada; Gopinathan, C. (Inorg. Chem. Div., Natl. Chem. Lab., Pune, 411 008, India). Indian J. Chem., Sect. A, 23A(11), 957-8 (English) 1984. CODEN: IJCADU. ISSN: 0376-4710.

Til2L12 (HL = (C6H5)2C(CH3)OH, HL1 = salicylaldehyde (I), 8-hydroxyquinoline (II), 2-hydroxyacetophenone, 2-hydroxy-4-methoxybenzophenone, BzN(Ph)OH, acetoacetanilide), Til2L32 (H2L2 = phenolphthalein,; HL3 = I, II, Me salicylate, acetylacetone, benzoylacetone, dibenzoylmethane, BzN(Ph)OH), and (C5H5)2Til2 (C5H5 = cyclopentadienyl) were prepd. from Til12(OPr-iso)2 and HL or Til32(OPr-iso)2 with H2L2, resp. The structures of the complexes were assigned on the basis of IR and 1H NMR spectral data. The complexes are monomeric and have an octahedral structure.

IT 23329-69-3

(reactions of, with diphenylethanol and phenolphthalein)

RN 23329-69-3 HCA

CN Titanium, bis(2-propanolato)bis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

QD411.J6

CC 78-7 (Inorganic Chemicals and Reactions)
IT 23329-69-3 59368-50-2 59368-51-3
(reactions of, with diphenylethanol and phenolphthalein)

L38 ANSWER 10 OF 48 HCA COPYRIGHT 1998 ACS

101:230699 Synthesis and properties of monocyclopentadienyltitanium compounds. Martin-Benito, R.; Jimenez-Aparicio, R.; Barral, M. C. (Fac. Cienc. Quin, Univ. Complut. Madrid, Madrid, Spain). J. Organomet. Chem. 269(3), 267-72 (English) 1984 CODEN: JORCAI. TSSN: 0022-328X.

The pentacoordinated complexes (RCp)TiCl2(acac) (R = H, Me, Ph2CH; RCp = R-substituted cyclopentadienyl, acac = acetylacetonate) were prepd. by photolysis of (RCp)2TiCl2 and acacH in THF and the hexacoordinated compds. (RCp)TiCl(acac)2 by the reaction of (RCp)2TiCl2 and acacH in the presence of Et3N in isobutyronitrile. The hexacoordinated complexes (RCp)TiClL2 (R = H, Me, Ph2CH; L = 8-oxyquinolate) were prepd. by the direct interaction of (RCp)2TiCl2 and 8-hydroxyquinoline in isobutyronitrile; these compds. can be obtained more quickly by photolysis of the same starting materials in THF soln.

IT 93347-14-9P 93364-87-5P

(prepn. and cond. of)

RN 93347-14-9 HCA

CN Titanium, chloro[(1,2,3,4,5-.eta.)-1-methyl-2,4-cyclopentadien-1-yl]bis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

PAGE 1-A

Me |

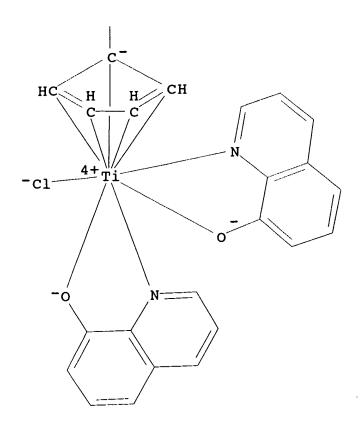
PAGE 2-A

RN 93364-87-5 HCA
CN Titanium, chloro[(1,2,3,4,5-.eta.)-1-(diphenylmethyl)-2,4cyclopentadien-1-yl]bis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

PAGE 1-A

 ${\tt CHPh_2}$

PAGE 2-A



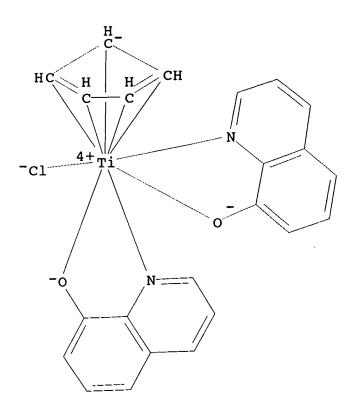
IT 31798-62-6P

(prepn. of)

RN 31798-62-6 HCA

CN Titanium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(8-quinolinolato-N1,08)-, stereoisomer (9CI) (CA INDEX NAME)





CC 29-10 (Organometallic and Organometalloidal Compounds)
IT 93346-96-4P 93347-11-6P 93347-12-7P 93347-13-8P
93347-14-9P 93364-87-5P 93364-88-6P
(prepn. and cond. of)
IT 31798-62-6P
(prepn. of)

L38 ANSWER 11 OF 48 HCA COPYRIGHT 1998 ACS

101:82965 New titanium(IV) chloroacetates. Awasarkar, P. A.;
Gopinathan, Sarada, Mrs.; Gopinathan, C. (Inorg. Chem. Div., Natl. Chem. Lab., Pune, 411 008, India). Indian J. Chem., Sect. A,
22A(12), 1076-7 (English) 1983. CODEN: IJCADU. ISSN: 0376-4710.

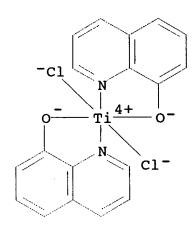
AB TiL2L12 (HL = ClCH2CO2H, HL1 = cyclopentadiene (HCp), acetylacetone
(Hacac); HL = Cl2CHCO2H, HL1 = HCp, Hacac, salicylaldehyde,
2-hydroxyacetophenone, 8-hydroxyquinoline; HL = Cl3CCO2H, HL1 = HCp,
salicylaldehyde) and Ti(O2CCCl3)4 were prepd. from TiL12Cl2 and NaL.
In TiL2L12 (HL1 .noteq. HCp), the acetate groups are monodentate to
form octrahedral complexes. No evidence for the assocn. of the mol.
was obtained. In TiCp2L2, the acetate groups are bidentate.

IT 16905-40-1

(reaction of, with dichloroacetic acid)

RN 16905-40-1 HCA

CN Titanium, dichlorobis(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 29

IT **16905-40-1** 91408-55-8

(reaction of, with dichloroacetic acid)

L38 ANSWER 12 OF 48 HCA COPYRIGHT 1998 ACS
99:175962 Some reactions of 8-quinolinol N-oxide with
bis(.eta.5-cyclopentadienyl)titanium dichloride. Goyal, K. C.;
Khosla, B. D. (Dep. Chem., Univ. Delhi, Delhi, 110 007, India). J.
Indian Chem. Soc., 60(4), 399-400 (English) 1983. CODEN: JICSAH.
ISSN: 0019-4522.

AB Treating a mixt. of (.epsilon.5-C5H5)2TiCl2 (I) and 8-quinolinol N-oxide (II) with NaNH2 in PhMe under reflux gave (.epsilon.5-C5H5)2TiLCl (L = N-oxido-8-quinolinolato). Treating a mixt. of I and II in MeCN with Et3N gave (.epsilon.5-C5H5)2TiL2 (same L).

IT 87612-44-0P

(prepn. of)

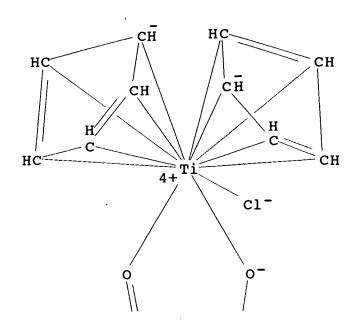
RN 87612-44-0 HCA

CN Titanium, chlorobis(.eta.5-2,4-cyclopentadien-1-yl)(8-quinolinol 1-oxidato-0,0')- (9CI) (CA INDEX NAME)

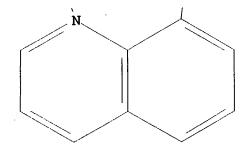


Rabago 08/872,659

PAGE 1-A

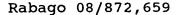


PAGE 2-A



CC 29-10 (Organometallic and Organometalloidal Compounds)
IT 87612-44-0P 87612-45-1P
(prepn. of)

L38 ANSWER 13 OF 48 HCA COPYRIGHT 1998 ACS
99:63207 Titanium(IV) and tin(IV) derivatives of salicylaldehyde
hydrazone and 2-hydroxyacetophenone hydrazone. Pardhy, Mrs. S. A.;



Gopinathan, Mrs. Sarada; Gopinathan, C. (Natl. Chem. Lab., Poona City, 411008, India). Synth. React. Inorg. Met.-Org. Chem., 13(4), 385-95 (English) 1983. CODEN: SRIMCN. ISSN: 0094-5714.

AB cis-R2SmL2 (HL = salicylaldehyde hydrazone (HSA), 2-hydroxyacetophenone hydrazone (HAcPA); R = Me, Bu, octyl) and Ph3SnL were prepd. from R2SnCl2 or Ph3SnCl, resp., and NaL. trans-TiL2Cl2 were prepd. from TiCl4 and HL. TiQ2(OPr-iso)2 (HQ = 8-hydroxyquinoline) and iso-Pr titanate reacted with HL to give TiL2Q2 and [TiL2O]2, resp. TiL12(OPr-iso)2 (HL' = salicylaldehyde) or TiL22(OPr-iso)2 (HL2 = acetylacetone, benzoylacetone, dibenzoylmethane) reacted with HSA or HAcPA to give TiL32 (H2L3 = Schiff bases derived from HSA or HAcPA and HL1 or HL2). These complexes were characterized by IR spectra.

IT 23329-69-3

(reaction of, with hydroxyacetophenone hydrazone and salicylaldehyde hydrazone)

RN 23329-69-3 HCA

CN Titanium, bis(2-propanolato)bis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

CC 78-7 (Inorganic Chemicals and Reactions) Section cross-reference(s): 29

IT 12103-39-8 17927-72-9 **23329-69-3** 59368-51-3 72439-63-5

(reaction of, with hydroxyacetophenone hydrazone and salicylaldehyde hydrazone)

L38 ANSWER 14 OF 48 HCA COPYRIGHT 1998 ACS

98:226899 Complexes of 8-quinolinol N-oxide with zirconium tetrachloride. Mittal, I. P.; Goyal, K. C.; Kaushik, N. K. (Dep. Chem., Univ. Delhi, Delhi, 110007, India). J. Inst. Chem. (India), 55(1), 29-32 (English) 1983. CODEN: JOICA7. ISSN: 0020-3254.

AB ZrCl4.2HL and ZrOCl2.2HL (HL = 8-quinolinol N-oxide) were prepd. from ZrCl4 and HL in ether or EtOH, resp. When a 1:2 ZrCl4-HL mixt. was refluxed in C6H6, ZrCl2L2 was obtained. ZrCl4.2HL and ZrCl2L2

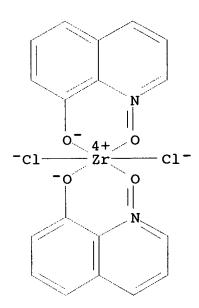
are 6-coordinate and ZrOCl2.2HL is 5-coordinate. In ZrCl4.2HL and ZrOCl2.2HL, HL is monodentate and coordinate through the N-O group. ZrCl4.2HL and ZrOCl2.2HL were characterized by thermogravimetry and IR spectra.

IT 85786-21-6P

(prepn. and IR spectrum of)

RN 85786-21-6 HCA

CN Zirconium, dichlorobis(8-quinolinol 1-oxidato-0,0')- (9CI) (CA INDEX NAME)



IT 85786-14-7P 85886-72-2P

(prepn., IR spectrum and thermogravimetry of)

RN 85786-14-7 HCA

CN Zirconium, dichlorooxobis(8-quinolinol 1-oxide-0,0')- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 85886-72-2 HCA

CN Zirconium, tetrachlorobis(8-quinolinol 1-oxide-0,0')- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CC 78-7 (Inorganic Chemicals and Reactions)

IT 85786-21-6P

(prepn. and IR spectrum of)

IT 85786-14-7P 85886-72-2P

(prepn., IR spectrum and thermogravimetry of)

L38 ANSWER 15 OF 48 HCA COPYRIGHT 1998 ACS

98:34674 Organoxytitanium(IV) and organotin(IV) derivatives of

saligenin. Pandit, S. K.; Gopinathan, Sarada; Gopinathan, C. (Inorg. Chem. Div., Natl. Chem. Lab., Poona City, 411 008, India). Indian J. Chem., Sect. A, 21A(7), 726-7 (English) 1982. CODEN: IJCADU. ISSN: 0376-4710.

AB Disodiosaligenin reacts with SnCl4 giving a dichloride; with diorganotin dichlorides, it forms diorganostannylsaligenin derivs. IR and NMR spectra indicate that the Ti compds., prepd. from bischelated diisopropoxytitaniums and saligenin, are 6-coordinate, while the Sn derivs. are 4-coordinate.

IT 23329-69-3

(reaction of, with saligenin)

RN 23329-69-3 HCA

CN Titanium, bis(2-propanolato)bis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 12103-39-8 17927-72-9 **23329-69-3** 59368-50-2

59368-51-3

(reaction of, with saligenin)

L38 ANSWER 16 OF 48 HCA COPYRIGHT 1998 ACS

95:72372 Complexes of titanium tetrachloride with 8-quinolinol N-oxide. Goyal, K. C.; Khosla, B. D. (Dep. Chem., Univ. Delhi, Delhi, 110 007, India). J. Indian Chem. Soc., 58(6), 617-19 (English) 1981. CODEN: JICSAH. ISSN: 0019-4522.

AB 8-Quinolinol N-oxide (HL) reacts with TiCl4 to give TiCl4.cntdot.HL and TiCl4.cntdot.2HL. Both adducts undergo thermal decompn. to give TiCl2L2 and finally TiO2. The complexes were characterized by chem. anal. and IR spectra. The IR spectra indicate that HL acts as a bidentate ligand in these complexes.

IT 78505-44-9P 78505-45-0P 78505-46-1P

(prepn. and thermal decompn. of)

RN 78505-44-9 HCA

CN Titanium, tetrachloro(8-quinolinol 1-oxide-0,0')-, (OC-6-32)- (9CI) (CA INDEX NAME)



RN 78505-45-0 HCA

CN Titanium, tetrachlorobis(8-quinolinol 1-oxide-0,0')- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 78505-46-1 HCA

CC 78-7 (Inorganic Chemicals and Reactions)

IT 78505-44-9P 78505-45-0P 78505-46-1P (prepn. and thermal decompn. of)

L38 ANSWER 17 OF 48 HCA COPYRIGHT 1998 ACS

94:113628 The isolation and characterization of some mixed ligand complexes of titanium(IV). Aly, Mohamed M.; Hassan, Mostafa K. (Fac. Sci., Assiut Univ., Assiut, Egypt). Ann. Chim. (Rome), 70(9-10), 463-70 (English) 1980. CODEN: ANCRAI. ISSN: 0003-4592. AB TiCl4(HL)2 (I; HL = 8-quinolinol) reacts with acetylacetone or

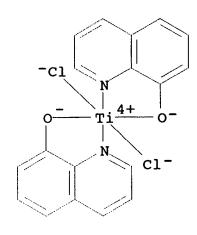
TiCl4(HL)2 (I; HL = 8-quinolinol) reacts with acetylacetone or salicylaldehyde to give TiCl2L2. I reacts with CF3CO2H to give Ti(O2CCF3)2L2 and with other haloacetates to give TiClL'L2 (HL' = CCl3CO2H, CHCl2CO2H). I and pyridine-2,6-dicarboxylic acid (H2L'') give TiCl(HL'')L2.HCl. A coordination no. of 8 is proposed for the TiClL'L2 and TiCl(HL'')L2.HCl complexes with Cl bridging ligands and bidentate L, L' and HL'' ligands.

IT 16905-40-1P 76770-41-7P 76770-43-9P 76779-21-0P

(prepn. of)

RN 16905-40-1 HCA

CN Titanium, dichlorobis(8-quinolinolato-.kappa.N1,.kappa.O8) - (9CI) (CA INDEX NAME)



RN 76770-41-7 HCA

Titanium, chlorobis(8-quinolinolato-N1,08)(trichloroacetato-0,0')-, homopolymer (9CI) (CA INDEX NAME) CN

CM

CRN 76770-40-6

CMF C20 H12 Cl4 N2 O4 Ti

CCI CCS

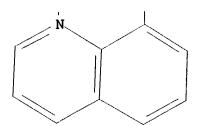
 $\sqrt{}$

Rabago 08/872,659

Page 107

PAGE 1-A

PAGE 2-A



RN 76770-43-9 HCA
CN Titanium, chloro[2,6-pyridinedicarboxylato(2-)-02,06]bis(8-quinolinolato-N1,08)-, monohydrochloride, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 76770-42-8

CMF C25 H15 Cl N3 O6 Ti . Cl H CCI CCS

● HCl

RN 76779-21-0 HCA CN Titanium, chloro(dichloroacetato-0,0')bis(8-quinolinolato-N1,08)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

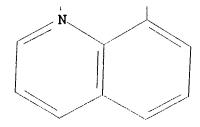
CRN 76779-20-9

CMF C20 H13 Cl3 N2 O4 Ti

CCI CCS

PAGE 1-A

PAGE 2-A



CC 78-7 (Inorganic Chemicals and Reactions)
IT 16905-40-1P 76770-41-7P 76770-43-9P
76771-15-8P 76779-21-0P
(prepn. of)

L38 ANSWER 18 OF 48 HCA COPYRIGHT 1998 ACS
94:15831 Bis-chelated titanium(IV) derivatives of triphenylsilanol,
diphenylsilanediol and triphenylcarbinol. Unny, I. R.; Gopinathan,

Sarada; Gopinathan, C. (Natl. Chem. Lab., Poona City, 411 008, India). Indian J. Chem., Sect. A, 19A(6), 598-9 (English) 1980. CODEN: IJCADU. ISSN: 0376-4710.

AB Bis-chelated Ti(IV) diisopropoxides, L2Ti(OPr)2, react with triphenylsilanol, diphenylsilanediol and triphenylcarbinol giving products L2Ti(OSiPh3)2, L2Ti(O2SiPh2) and L2Ti(OCPh3)2 resp. The ligands (L) used are salicylaldehyde, acetylacetone, 8-hydroxyquinoline, acetoacetanilide and 2-hydroxy-4-methoxybenzophenone. Ti(OPr)4 reacts with triphendylcarbinol giving Ti(OCPh3)4. The new titanosiloxanes have good thermal stabilities.

IT 75576-95-3

(reaction of, with alcs.)

RN 75576-95-3 HCA

CN Titanium, dipropoxybis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

CC 29-10 (Organometallic and Organometalloidal Compounds)
IT 3087-37-4 21474-51-1 50363-05-8 75576-94-2 **75576-95-3**75576-96-4
(reaction of, with alcs.)

L38 ANSWER 19 OF 48 HCA COPYRIGHT 1998 ACS

92:198492 Bromides and phenoxides of bis(cyclopentadienyl)chelate derivatives of zirconium. Brainina, E. M.; Minacheva, M. Kh. (Inst. Elementoorg. Soedin., Moscow, USSR). Izv. Akad. Nauk SSSR, Ser. Khim. (2), 410-13 (Russian) 1980. CODEN: IASKA6. ISSN: 0002-3353.

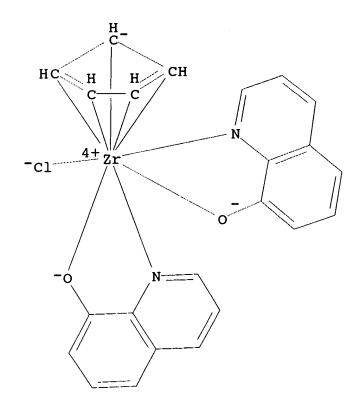
AB (.eta.5-C5H5)2ZrLX (LH = BzCH2Ac, Bz2CH2, (L1H), 8-hydroxyquinoline; X = Br, PhO) were prepd. in 41-81% yields. Thus, treating [(.eta.5-C5H5)2ZrBr]2O with L1H gave 44% (.eta.5-C5H5)2ZrL1Br.cntdot.H2O.

IT 12114-15-7P 73655-94-4P

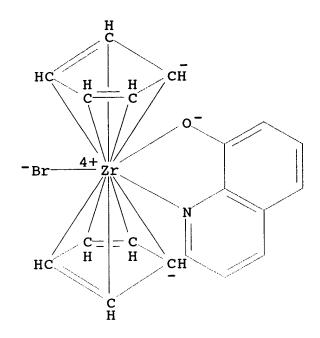
(prepn. of)

RN 12114-15-7 HCA

CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(8-quinolinolato-N1,08)-, stereoisomer (9CI) (CA INDEX NAME)



RN 73655-94-4 HCA CN Zirconium, bromobis(.eta.5-2,4-cyclopentadien-1-yl)(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)
IT 12114-15-7P 39475-31-5P 73655-93-3P 73655-94-4P
73655-95-5P 73655-96-6P 73655-97-7P 73655-98-8P 73655-99-9P
73667-87-5P
(prepn. of)

ANSWER 20 OF 48 HCA COPYRIGHT 1998 ACS L38 The reactions of tert-butyl isocyanide with halides of 92:76627 titanium(IV), hafnium(IV), vanadium(III), niobium(IV), molybdenum(V) and tungsten(VI); insertion into metal-halogen bonds and ligand displacement reactions. Behnam-Dehkordy, Mahbobeh; Crociani, Bruno; Nicolini, Marino; Richards, Raymond L. (Sch. Mol. Sci., Univ. Sussex, Brighton, BN1 9QJ, Engl.). J. Organomet. Chem., 181(1), 69-80 (English) 1979. CODEN: JORCAI. ISSN: 0022-328X. t-BuNC inserts into a metal-halogen bond of TiCl4, HfCl4, VCl3 and AB [NbCl4(THF)2] to give [TiCl3(C(Cl)NBu-t)(CNBu-t)]2, $[HfCl3{C(Cl)NBu-t}(CNBu-t)]2$, $[VCl2{(C(Cl)NBu-t}(CNBu-t2)]2$ and [NbCl3{C(Cl)NBu-t}(CNBu-t)]2,resp. [MoCl4(THF)2] and WCl6 do not give inserted products, but rather [MoCl3(CNBu-t)3]Cl and trans-[WCl4(CNBu-t)2]. Treatment of these inserted products and $[MX4\{C(X)NBu-t\}(CNBu-t)2]$ (M = Nb or Ta, X = Cl or Br) with Li quinolin-8-olate (Li[8-quin]), Na diethyldithiocarbamate (Na[dtc]) or Ph2PCH2CH2PPh2 (dppe) causes displacement of terminal t-BuNC in all cases and in some cases of the iminoethyl ligand as well. obtained are the complexes [TiCl2{C(Cl)NBu-t}(8-quin)], [TiCl4(dppe)], [TiCl2(dtc)2], [HfCl2(C(Cl)NBu-t)(8-quin)], [HfCl3{C(Cl)NBu-t}(dppe)], [Hf(dtc)4], [VCl{C(Cl)NBu-t}(8-quin)], [V(dtc)4], [NbCl2{C(Cl)NBu-t}(8-quin)]2, [NbCl{C(Cl)NBu-t}(dtc)2]2, $[MX3\{C(X)NBu-t\}(8-quin)]$ (M = Nb or Ta, X = Cl or Br),

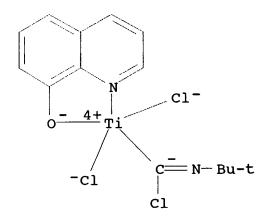
[NbX2{C(X)NBu-t}(dtc)2] and [TaX3{C(X)NBu-t}(dtc)]2.Ta2Br10 gives TaB3(dtc)2 on treatment with Na[dtc].

IT 72637-85-5P 72637-86-6P

(prepn. and spectral properties of)

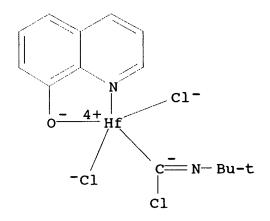
RN 72637-85-5 HCA

CN Titanium, dichloro[chloro[(1,1-dimethylethyl)imino]methyl](8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)



RN 72637-86-6 HCA

CN Hafnium, dichloro[chloro[(1,1-dimethylethyl)imino]methyl](8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)



29-10 (Organometallic and Organometalloidal Compounds) CC 58019-14-0P 57974-90-0P IT 12406-70-1P 57974-86-4P 57974-88-6P 71737-46-7P 72637-85-5P 72637-86-6P 72637-89-9P 72637-90-2P 72637-93-5P 72637-87-7P 72637-88-8P 72637-98-0P 72638-00-7P 72637-95-7P 72637-96-8P 72637-94-6P 72638-01-8P

(prepn. and spectral properties of)

L38 ANSWER 21 OF 48 HCA COPYRIGHT 1998 ACS
91:163068 Synergistic compositions and method of use to treat
inflammation. Klein, Robert W.; Nuss, George W., Jr. (USA). U.S.
US 4163783 790807, 5 pp. (English). CODEN: USXXAM. APPLICATION:
US 77-835595 770922.

GI

AB A synergistic topical inflammation inhibiting compn. contains a nonsteroid inflammation inhibitor and I (M = Zn, Fe, Mg, Sn, Cd, Zr, or alkali and alk. earth metals; Y = anion; t = 1 or 2). A topical cream (100 g) was prepd. contg. I (M = Ca, Y = Cl, t = 2) [43143-10-8] 1 g and 1-(p-chlorobenzoyl)-5-methoxy-2-methylindole-3-acetic acid [53-86-1] 0.3 g.

IT 70675-90-0

(synergistic topical inflammation inhibiting compns. contg.)

RN 70675-90-0 HCA

CN Zirconium, tetrachloro[2,2'-dithiobis[pyridine] 1,1'-dioxide-0,0',S]-(9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IC A61K031-44; A61K031-555

NCL 424245000

CC 63-6 (Pharmaceuticals)

IT 43143-10-8 70675-89-7 **70675-90-0** 70675-91-1 70848-99-6 70849-00-2 70849-02-4 71724-05-5 (synergistic topical inflammation inhibiting compns. contg.)

L38 ANSWER 22 OF 48 HCA COPYRIGHT 1998 ACS

91:97345 Configurational rearrangements in cis-M(AA)2X2, cis-M(AA)2XY, and cis-M(AB)2X2 complexes. 6. Bis(chelate)bis(2,6-diisopropylphenoxy)titanium systems (chelate = acetylacetonate, 8-hydroxyquinolinate, and 8-hydroxyquinaldinate). Bickley, Douglas G.; Serpone, Nick (Dep. Chem., Concordia Univ., Montreal, PQ, H3G 1M8, Can.). Inorg. Chem., 18(8), 2200-4 (English) 1979. CODEN: INOCAJ. ISSN: 0020-1669.

For a series of bis(chelate), bis(2,6-diisopropylphenoxy)titanium complexes [chelate = acetylacetonate (acac), 8-hydroxyquinolinate (ox), and 8-hydroxyquinlinate (quin)] an NMR total line shape anal. of iso-Pr Me group exchange (inversion) is reported, along with data for acac Me group exchange for the corresponding acac complex. Activation energies (kcal/mol) and entropies (entropy units), in

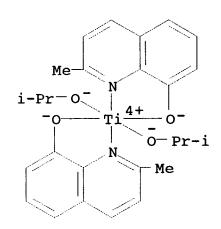
m-dichlorobenzene solns., for inversion are, resp., 6.3 .+-. 1.7 and -36.5 .+-. 5.7 (acac), 14.7 .+-. 0.8 and -9.7 .+-. 2.2 (quin), and 21.2 .+-. 1.3 and 2.2 .+-. 3.3 (ox). For acac Me group exchange, the corresponding kinetic data are (in m-dichlorobenzene soln.) 13.8 .+-. 0.3 and -10.6 .+-. 1.0. Dramatic differences between kinetic parameters suggest that the ox and quin complexes possess a different rearrangement route than that for the acac complex. On the assumption that the ox and quin complexes retain the same structure in solid and soln. phases, the iso-Pr Me group exchange is identified as resulting from the process cis(phenoxy),cis(n),trans(0)-.DELTA.(.lambda.) .dblarw. cis(phenoxy)cis(n),trans(0)-.lambda.(.DELTA.). This rearrangement stereochem. can only be generated via a Ti-n bond-rupture mechanism occurring through a trigonal-bipyramidal axial intermediate.

IT 33888-32-3P

(prepn. and substitution reaction of)

RN 33888-32-3 HCA

CN Titanium, bis(2-methyl-8-quinolinolato-N1,08)bis(2-propanolato)(9CI) (CA INDEX NAME)



CC 67-3 (Catalysis and Reaction Kinetics)
Section cross-reference(s): 73

IT 33888-32-3P

(prepn. and substitution reaction of)

L38 ANSWER 23 OF 48 HCA COPYRIGHT 1998 ACS
91:78909 Compositions for treating inflammation. Klein, Robert W.
(Rorer, William H., Inc., USA). U.S. US 4152431 790501, 5 pp.
(English). CODEN: USXXAM. APPLICATION: US 77-835594 770922.
GI

Topical antiinflammatory compns. contain bis(2-pyridyl-1-oxide) disulfide (I) [3696-28-4] or I.MYt when M = Zn, Fe, Mg, Sn, Cd, Zr, or alkali or alk. earth metals and Y is an anion and t = 1 or 2. Topical compns. such as creams, ointments, or aerosols were prepd. contg. I derivs. such as I.MgSO4 [70849-05-7] or I.CaCl2 [70849-06-8].

IT 70849-04-6

(inflammation inhibiting topical compns. contg.)

RN 70849-04-6 HCA

IC A61K031-44; A61K031-555

NCL 424245000

CC 63-6 (Pharmaceuticals)

IT 3696-28-4 70848-99-6 70849-00-2 70849-01-3 70849-02-4 70849-03-5 **70849-04-6** 70849-05-7 70849-06-8 71016-06-3 (inflammation inhibiting topical compns. contg.)

L38 ANSWER 24 OF 48 HCA COPYRIGHT 1998 ACS

91:62729 Antiinflammatory agent. Klein, Robert Warren; Nuss, George Werner, Jr. (Rorer, William H., Inc., USA). Ger. Offen. DE 2840684 790405, 24 pp. (German). CODEN: GWXXBX. PRIORITY: US 77-835594 770922.

GI

AB A topical antiinflammatory compn. contains dithiobis(2-pyridine 1-oxide) (I) [3696-28-4] or a complex L2MXn (L = I; M = Zn, Fe, Mg, Sn, Cd, Zr, alkali metal, alk. earth metal; X = anion; n = 1, 2) and optionally another inflammation inhibitor. Thus an ointment was prepd. from I.CaCl2 [70675-92-2] 2 and hydrocortisone (II) [50-23-7] 0.05 g. A mixt. of I.MgCl2 [43143-11-9] 4 mg and II 1 mg caused 67.5% inhibition of croton oil-induced edema in mice.

IT 70675-90-0

(topical antiinflammatory compn. contg.)

Rabago 08/872,659

RN 70675-90-0 HCA

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IC A61K031-44; A61K031-095; A61K031-57

CC 63-6 (Pharmaceuticals)

IT 3696-28-4 43143-11-9 70675-87-5 70675-88-6 70675-89-7

70675-90-0 70675-91-1 70675-92-2

(topical antiinflammatory compn. contg.)

L38 ANSWER 25 OF 48 HCA COPYRIGHT 1998 ACS

Ι

90:142170 Synergistic compositions. Klein, Robert W.; Nuss, George W., Jr. (Rorer, William H., Inc., USA). U.S. US 4137311 790130, 6 pp. (English). CODEN: USXXAM. APPLICATION: US 77-835596 770922.

GΙ

$$s_2$$
 0 MY_t

AB Antiinflammatory compns. for treating skin are prepd. comprising synergistic combination of a corticosteroid and bis(2-pyridyl-1-oxide) metal salts (I, M = metal, Y = anion, t = 1 or 2). Thus, an antiinflammatory dosage of 4 mg bis(2-pyridyl-1-oxide)disulfide magnesium sulfate [43143-11-9] and 1 mg hydrocortisone [50-23-7] produced 67.5% inhibition of croton oil-induced edema to mouse's ear. Dermatol. cleansing cakes and powders were prepd. contg. these synergistic mixts.

IT 69697-31-0

(antiinflammatory synergistic compns. contg. corticosteroids and)

RN 69697-31-0 HCA

CN Zirconium, tetrachloro[2,2'-dithiobis[pyridine] 1,1'-dioxide]-, (OC-6-33)- (9CI) (CA INDEX NAME)

IC A61K031-56

NCL 424240000

CC 63-6 (Pharmaceuticals)

IT 43143-10-8 43143-11-9 43143-12-0 69697-29-6 69697-30-9

69697-31-0 69697-32-1

(antiinflammatory synergistic compns. contg. corticosteroids and)

L38 ANSWER 26 OF 48 HCA COPYRIGHT 1998 ACS

90:33240 Studies on 8-quinolinol-N-oxides and some of their metal chelates. Ghuge, K. D.; Umapathy, P.; Sen, D. N. (Natl. Chem. Lab., Poona City, India). J. Indian Chem. Soc., 55(9), 864-8 (English) 1978. CODEN: JICSAH. ISSN: 0019-4522.

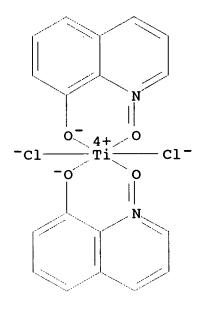
AB Several metal chelates of 8-quinolinol N-oxide with Cu(II), Be, Mn(II), Sn(II), Fe(III), Cr(III), Al, Sn(IV), Ti(IV), UO22+, VO2+ and MoO22+ and also Cu(II), Fe(III), VO2+, and VO22+ chelates of 5-nitro-, 5,7-dinitro- and 5,7-dibromo-8-quinolinol N-oxide, were prepd. in pure state. These chelates are characterized by their elemental analyses, IR, UV-visible spectral, and magnetic susceptibility data wherever possible. The ligands act as bidentate, chelating agents, coordinating through the NO O and the phenolic hydroxyl O atoms. IR evidence is provided for the monodentate neutral character of the ligands in Sn(II) and Sn(IV) complexes. Deuteration studies were also made.

IT 68811-33-6P 68811-34-7P

(prepn. of)

RN 68811-33-6 HCA

CN Titanium, dichlorobis(8-quinolinol 1-oxidato-0,0')- (9CI) (CA INDEX NAME)



RN 68811-34-7 HCA CN Titanium, diethoxybis(8-quinolinol 1-oxidato-0,0')- (9CI) (CA INDEX NAME)

78-7 (Inorganic Chemicals and Reactions) CC 68811-10-9P 68811-11-0P 68811-12-1P IT 52519-37-6P 52519-38-7P 68811-24-5P 68811-25-6P 68811-26-7P 68811-27-8P 68811-28-9P 68811-31-4P 68811-32-5P 68811-30-3P 68811-29-0P 68811-33-6P 68811-34-7P 68811-35-8P

68811-36-9P 68811-37-0P 68824-12-4P (prepn. of)

L38 ANSWER 27 OF 48 HCA COPYRIGHT 1998 ACS

89:24870 Synthesis of polymers based on chelate titanium compounds.
Nogaideli, A. I.; Mikhailov, M. B.; Pichkhadze, Sh. V. (Tbilis. Gos. Univ., Tiflis, USSR). Izv. Akad. Nauk Gruz. SSR, Ser. Khim., 3(4), 344-9 (Russian) 1977. CODEN: IGSKDH.

Four copolymers were prepd. by polycondensation of bis(benzoylacetonato)bis(butanolato)titanium and bis(butanolato)bis(8-quinolinolato)titanium (I) with hydroquinone and 2,2-bis(4-hydroxyphenyl)propane (II). The reactions were conducted at 170.degree. and 1:1 molar ratio of the comonomers. The structure of the copolymers was established on the basis of evolution of BuOH during the polymn., elemental anal., and IR spectra. The red-brown copolymers were sol. in dioxane, DMF, and THF. The presence of I and II units in the copolymers shifted their glass transition to higher temps.

IT 66690-01-5P 66690-02-6P

(prepn., properties and structure of)

RN 66690-01-5 HCA

CN Titanium, dibutoxybis(8-quinolinolato-N1,08)-, polymer with 1,4-benzenediol (9CI) (CA INDEX NAME)

CM 1

CRN 17034-82-1 CMF C26 H30 N2 O4 Ti CCI CCS

CM 2

CRN 123-31-9 CMF C6 H6 O2

RN 66690-02-6 HCA

CN Titanium, dibutoxybis(8-quinolinolato-N1,08)-, polymer with 4,4'-(1-methylethylidene)bis[phenol] (9CI) (CA INDEX NAME)

CM 1

CRN 17034-82-1

CMF C26 H30 N2 O4 Ti

CCI CCS

CM 2

CRN 80-05-7

CMF C15 H16 O2

CC 35-3 (Synthetic High Polymers)

IT 66689-99-4P 66690-00-4P **66690-01-5P 66690-02-6P**66690-04-8P 66690-06-0P 66690-08-2P 66690-10-6P
(prepn., properties and structure of)

L38 ANSWER 28 OF 48 HCA COPYRIGHT 1998 ACS
87:53910 Thermal stability of some chelate titanosiloxane oligomers.
Krivonishchenko, V. V.; Suvorov, A. L.; Malyarenko, A. V. (Inst.
Khim., Sverdlovsk, USSR). Vysokomol. Soedin., Ser. B, 19(5), 382-6
(Russian) 1977. CODEN: VYSBAI.
GI

The title polymers of structure BuO(TiR2OSiMe2C6H4SiMe2O)nH (R = I-VIII) with coordinatively satd. Ti atoms in the main chain (R = III-VIII), in contrast to alkoxy- or aryloxytitanosiloxanes (R = I-II), were resistant to thermal disproportionation and their oxidative thermal stability was detd. by the structure of the chelated ligand at the Ti. The investigated polymers were prepd. by condensation of p-(HOSiMe2)C6H4 with (BuO)2TiR2, and their stability was compared with that of oligomeric HO(TiR2O)nH (R = III-V, n = 2-3), modeling the chain units of the polymers.

IT 63533-38-0 63559-75-1

(oxidative thermal stability of)

RN 63533-38-0 HCA

CN Titanium, dibutoxybis(8-quinolinolato-N1,08)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

0

CRN 17034-82-1

CMF C26 H30 N2 O4 Ti CCI CCS

RN 63559-75-1 HCA

CN Titanium, dibutoxybis(8-quinolinolato-N1,08)-, polymer with 1,4-phenylenebis[dimethylsilanol] (9CI) (CA INDEX NAME)

CM 1

CRN 17034-82-1

CMF C26 H30 N2 O4 Ti

CCI CCS

CM 2

CRN 2754-32-7

CMF C10 H18 O2 Si2

CC 36-4 (Plastics Manufacture and Processing)
IT 63525-74-6 63525-76-8 63533-31-3 63533-33-5 63533-35-7
63533-36-8 63533-37-9 63533-38-0 63533-39-1
63559-75-1 63587-27-9
(oxidative thermal stability of)

L38 ANSWER 29 OF 48 HCA COPYRIGHT 1998 ACS
84:74865 Polychelatotitanoarylenesiloxanes. Suvorov, A. L.; Malykhin,
A. P.; Malyarenko, A. V. (Ural Institute of Chemistry, USSR).
U.S.S.R. SU 492524 751125 From: Otkrytiya, Izobret., Prom.
Obraztsy, Tovarnye Znaki 1975, 52(43), 64-5. (Russian). CODEN:
URXXAF. APPLICATION: SU 73-1948565 730712.

The title compds. with improved thermal and oxidative stability were prepd. by polycondensing an unsatd. bis(chelato)dialkoxytitanium, e.g. bis(7-ally1-8-quinolyloxy)dibutoxytitanium [58249-06-2], bis(2-methacryloy1-4-methylphenoxy)dibutoxytitanium [58218-70-5], bis(2-ally1-6-carbethoxyphenoxy)diethoxytitanium [58218-71-6], or bis(2-carballyloxyphenoxy)diethoxytitanium [58218-72-7] with arom. bis(hydroxydiorganosilyl) compds. at 40-80.degree. in Et20 [60-29-7] as the solvent.

IC CO8G

CC 35-3 (Synthetic High Polymers)

L38 ANSWER 30 OF 48 HCA COPYRIGHT 1998 ACS 84:68867 Chemistry of phenoxo complexes. III. Preparation and

characterization of some bis(chelato)bis(phenoxo)titanium(IV)
complexes. Harrod, J. F.; Taylor, K. R. (Chem. Dep., McGill Univ.,
Montreal, Que., Can.). Inorg. Chem., 14(7), 1541-5 (Enlis) 195.
CODEN: INOCAJ.

AB A large no. of bis(chelato)bis(phenoxo)titanium(IV) complexes were prepd. by metathesis between a phenol and bis(chelato)bis(alkoxo)titanium(IV), where chelato = acetylacetonato, 8-quinolinolato, or 2-methyl-8-quinolinolato and alkoxo = n butoxo or isopropoxo. In spite of the very wide range of electronic and steric properties of the phenoxy substituents, only complexes of cis stereochem. were obsd., and there seems little likelihood that complexes of this type can be induced to adopt a trans configuration. The dipole moments (D) and the relative chem. shifts (.DELTA..delta.) of the methine protons for a no. of



acetylacetonate complexes were measured. No systematic trends in the variation of .DELTA..delta. either with D or with the .rho.parameters of the phenoxy ligands were obsd.

IT 33888-32-3 54516-87-9

(pren. and dipole moment of)

RN 33888-32-3 HCA

CN Titanium, bis(2-methyl-8-quinolinolato-N1,08)bis(2-propanolato)(9CI) (CA INDEX NAME)

RN 54516-87-9 HCA CN Titanium, dibutoxybis(2-methyl-8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

IT 17034-82-1P

(prepn. and dipole moments of)

RN 17034-82-1 HCA

CN Titanium, dibutoxybis(8-quinolinolato-N1,08) - (9CI) (CA INDEX NAME)

IT 23329-69-3P

(prepn. of)

RN 23329-69-3 HCA

CN Titanium, bis(2-propanolato)bis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 73

IT 33888-31-2 33888-32-3 38781-12-3 54516-87-9

(pren. and dipole moment of)

IT 17034-82-1P 33939-16-1P 54516-88-0P 54516-91-5P

54516-92-6P 54548-69-5P

(prepn. and dipole moments of)

IT 23329-69-3P 38781-13-4P 54516-89-1P 54516-90-4P

54516-94-8P 54516-95-9P 54516-96-0P 54516-99-3P 54517-01-0P (prepn. of)

L38 ANSWER 31 OF 48 HCA COPYRIGHT 1998 ACS

83:70688 Preparation of quinolin-8-olates of titanium(III). Frazer, M. J.; Taylor, F. B.; Wilkins, T. A. (Dep. Chem., Polytech. North

London, London, Engl.). J. Inorg. Nucl. Chem., 37(3), 675-7 (English) 1975. CODEN: JINCAO.

Quinolin-8-ol (LH) with .alpha.-TiCl3 and TiBr3 in MeCN gave the quinolinolates TiXL2 (I; X = Cl, Br) and the adduct TiCl3.2LH (II). AΒ TiL3 with TiBr3 in MeCN also gave TiBrL2. Redn. of TiClL3 by Na in PhMe and of TiCl2L2 by K in C6H6 gave TiL3 and TiClL2, resp. Reaction of I and II with dry 02 gave (TiXL2)20 and [TiCl3(LH)2]20, resp.

IT 56212-10-3P 56212-12-5P 56212-13-6P 56212-15-8P

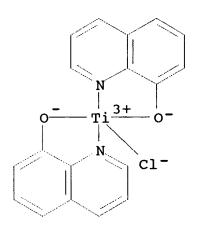
(prepn. of)

56212-10-3 HCA RN

Titanium, chlorobis(8-quinolinolato-N1,O8)-, homopolymer (9CI) CN INDEX NAME)

CM 1

CRN 56212-09-0 C18 H12 Cl N2 O2 Ti CMF CCI CCS



RN56212-12-5 HCA

Titanium, bromobis(8-quinolinolato-N1,08)-, homopolymer (9CI) CN INDEX NAME)

CM 1

CRN 56212-11-4

C18 H12 Br N2 O2 Ti CMF

CCI CCS

RN 56212-13-6 HCA CN Titanium, dichloro-.mu.-oxotetrakis(8-quinolinolato-N1,08)di- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 56212-15-8 HCA CN Titanium, dibromo-.mu.-oxotetrakis(8-quinolinolato-N1,08)di- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

IT 16905-40-1

(redn. of, by potassium)

RN 16905-40-1 HCA

CN Titanium, dichlorobis(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)

IT 17442-90-9

(redn. of, by sodium)

RN 17442-90-9 HCA
CN Titanium, chlorotris(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI)
(CA INDEX NAME)

CC 78-7 (Inorganic Chemicals and Reactions)

IT 56212-10-3P 56212-12-5P 56212-13-6P

56212-14-7P 56212-15-8P

(prepn. of)

IT 16905-40-1

(redn. of, by potassium)

IT 17442-90-9

(redn. of, by sodium)

L38 ANSWER 32 OF 48 HCA COPYRIGHT 1998 ACS

83:70081 Redistribution reactions in the ion source of a mass spectrometer of complexes of titanium(IV), tin(IV), and germanium(IV) with 8-quinolinolato and halo or ethoxy ligands.

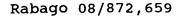
Barrett, C. G. R.; Charalambous, J.; Copperthwaite, R. G.; Frazer, M. J. (Polytech. North London, London, Engl.). Org. Mass Spectrom., 10(2), 146-54 (English) 1975. CODEN: ORMSBG.

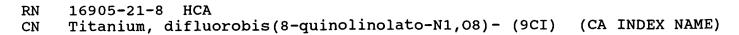
AB In the mass spectra of MX2R2 (M = Ge, Sn, Ti, X = F, Cl, Br, I, and

AB In the mass spectra of MX2R2/(M = Ge, Sn, Ti, X = F, Cl, Br, I, and R = 8-quinolinolato) and of Ti(OEt)4-nRn (n = 1, 2) redistribution reactions occurred to give ions of the type MX3R and MXR3. These reactions were confirmed by the variation in relative intensities of the peaks with insertion temp. and residence time of the sample in the spectrometer. The main fragmentation of MX2R2 were loss of X or whole quinolinol radicals, reflecting the metal-halogen bond strength and the tendency of the metal to exist in low oxidn. states. Decompn. of Ti(OEt)3R and Ti(OEt)2R2 involved loss of intact ligand radicals, whereas Ti(OEt)4 also eliminated ligand fragments.

IT 16905-21-8 16905-40-1 16905-41-2 23329-68-2 56531-00-1

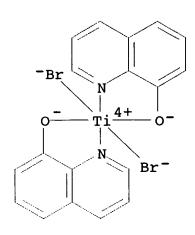
(mass spectrum of)





RN 16905-40-1 HCA CN Titanium, dichlorobis(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)

RN 16905-41-2 HCA CN Titanium, dibromobis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)



RN 23329-68-2 HCA CN Titanium, diethoxybis(8-quinolinolato-N1,O2)- (9CI) (CA INDEX NAME)

RN 56531-00-1 HCA CN Titanium, triethoxy(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

76-11 (Electric Phenomena) CC 3087-36-3 **16905-21-8** 16905-23-0 16905-24-1 IT 16905-26-3 16905-35-4 **16905-40-1** 16905-25-2 16925-43-2 23329-68-2 16905-41-2 56531-00-1 (mass spectrum of)

ANSWER 33 OF 48 HCA COPYRIGHT 1998 ACS

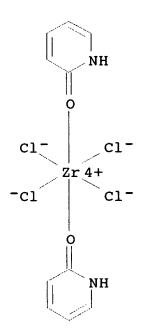
79:119046 Heats of addition of pyridine and its derivatives to zirconium tetrachloride. Konunova, Ts. B.; Frunze, M. F. (Kishinev. Politekh. Inst. im. Lazo, Kishinev, USSR). Zh. Neorg. Khim., 18(7), 1800-5 (Russian) 1973. CODEN: ZNOKAQ.

Heats of adduct formation of ZrCl4 with .alpha.-, .beta.-, AΒ o-picoline, .alpha.,.alpha.'-lutidine, .alpha.- and .beta.-chloropyridine, .gamma.-aminopyridine, .alpha.-amino-5bromopyridine, .alpha.-pyridone, .beta.-benzoylpyridine, and .alpha.,.alpha.'-dipyridyl were detd. The heats of addn. of gaseous pyridine derivs. to anhyd. ZrCl4 are calcd. The heats become increasingly more neg. with an increasing pKa value of the amines.

IT 37266-35-6P

(formation and heat of soln. of, in aq. hydrochloric acid) 37266-35-6 HCA RN

Zirconium, tetrachlorobis(2(1H)-pyridinone)- (9CI) (CA INDEX NAME) CN



69-1 (Thermodynamics, Thermochemistry, and Thermal Properties) CC Section cross-reference(s): 78

42720-65-0P 38294-43-8P 17100-06-0P 37266-35-6P IT42720-66-1P 42769-05-1P 46946-20-7P 46946-24-1P 46946-26-3P 51176-89-7P 51176-90-0P 51176-92-2P (formation and heat of soln. of, in aq. hydrochloric acid)

L38 ANSWER 34 OF 48 HCA COPYRIGHT 1998 ACS

78:111503 Organocyclotitanosiloxanes. Pakhomov, V. I.; Levin, B. B.; Fomina, N. I.; Maizner, I. M.; Malyukova, F. Sh.; Shesternina, L. A.; Portnaya, N. Kh. U.S.S.R. SU 362018 721213 From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1972, 50(2), 53. (Russian). CODEN: URXXAF. APPLICATION: SU 710121.

AB Organocyclotitanosiloxanes were prepd. by treating 3 equiv. of Ph2Si(OH)2 with 1 equiv. of bis(8-quinolinoxy)dibutoxytitanium in a solvent at 150-80.degree..

IT 41310-05-8

(reaction of, with dihydroxydiphenylsilane)

RN 41310-05-8 HCA

CN Titanium, dibutoxybis(8-quinolinolato-0)- (9CI) (CA INDEX NAME)

IC CO7F

CC 29-6 (Organometallic and Organometalloidal Compounds)

IT 41310-05-8

(reaction of, with dihydroxydiphenylsilane)

L38 ANSWER 35 OF 48 HCA COPYRIGHT 1998 ACS
77:172052 Synthesis of complex compounds of zirconium and hafnium tetrahalides with primary amines. Konunova, Ts. B.; Frunze, M. F. (USSR). Tr. Tekhnol. Fak., Kishinev. Politekh. Inst., No. 24, 75-9 From: Ref. Zh., Khim. 1972, Abstr. No. 5V93 (Russian) 1971.
AB From Ref. Zh., Khim. 1972, Abstr. No. 5V93. The addn. of amine solns. in EtOAc to solns. of ZrCl4 in EtOAc gave the adducts ZrCl4.nL.mEtOAc, where n, L, and m are: 2, py, and 1 (I); 2, .alpha.-picoline (pic), and 0.5 (II); 2, .beta.-pic, and 0.5; 2,

.gamma.-pic, and 0.5; 1.5, 3-benzylpyridine, and 1 (III); 2, 3-chloropyridine, and 0, 2, .alpha.-pyridone, and 0. I-III

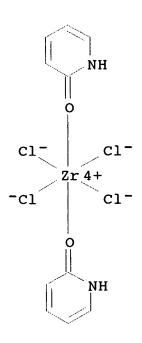
completely lost EtOAc at 100.degree.. The adducts HfCl4.2L, where L = py and .alpha.-pic, were also sepd. from solns. in EtOAc. ZrCl4.2(iso-PrNH2).EtOAc and ZrCl4.4EtNH2.1.5EtOAc were obtained from solns. of ZrCl4 in EtOAc and solns. of amines in ether. ZrCl4 adducts with PhNH2 derivs. were sepd. from ether solns. These complexes were ZrCl4.nL, where n and L are: 2 and C7H8N(sic); 4 and C7H8N(sic); 4 and p-toluidine.

IT 37266-35-6P

(prepn. of)

RN 37266-35-6 HCA

CN Zirconium, tetrachlorobis(2(1H)-pyridinone)- (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)
IT 17100-02-6P 37266-35-6P 37266-85-6P 38293-32-2P
38293-33-3P 38293-34-4P 38293-35-5P 38294-43-8P 38296-88-7P
38442-04-5P 38442-05-6P 38448-78-1P
(prepn. of)

L38 ANSWER 36 OF 48 HCA COPYRIGHT 1998 ACS
77:36006 Organosilicon elastic compositions. Severnyi, V. V.;
Varlamova, N. V.; Minsker, E. I. Fr. FR 2076539 711119, 13 pp.
(French). CODEN: FRXXAK. APPLICATION: FR 70-1792 700119.

AB Elastomeric organosilicon compns. having improved heat resistance,
water resistance, and adhesion to metal substrates were prepd.
comprising .alpha.,.omega.-dihydroxypoly(diorganosiloxanes),
Si-contg. hardeners, and metal chelates. Thus, a homogeneous mixt.
of .alpha.,.omega.-dihydroxypoly(dimethylsiloxane), ZnO,
bis(acetoacetonate) dibutoxytitanium [16902-59-3], tetraethoxysilane
[78-10-4], and diethylaminomethyltriethoxysilane [15180-47-9] was

applied on a metal or org. glass substrate and cured at ambient temp. and 60% relative humidity to give an adherent film. Among the other metal chelates used were acetylacetatodiisopropoxyaluminum [19223-59-7] and bis(8-hydroxyquinoline) dibutoxytitanium [17034-82-1].

IT 17034-82-1

CN

(vulcanizing agents, contg. silanes, for silicone rubber)

RN 17034-82-1 HCA

Titanium, dibutoxybis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

IC C08G; C09K

CC 38-9 (Elastomers, Including Natural Rubber)

IT 15710-92-6 16902-59-3 17034-82-1 19223-59-7

38856-15-4

(vulcanizing agents, contq. silanes, for silicone rubber)

L38 ANSWER 37 OF 48 HCA COPYRIGHT 1998 ACS

76:142027 Physical properties of poly(organosiloxanes). II. Nonlinear and irregular poly(elementorganosiloxanes). Andrianov, K. A.; Slonimskii, G. L.; Zhdanov, A. A.; Levin, V. Yu.; Godovskii, Yu. K.; Moskalenko, V. A. (Inst. Organo-Elem. Compd., Moscow, USSR). J. Polym. Sci., Part A-1, 10(1), 23-43 (English) 1972. CODEN: JPLCAT.

AB Metal-contg. silicone rubber was prepd. by polymn. of siloxanes with aluminum butoxide [3085-30-1], tributoxy(8-quinolinolato)titanium [

14843-25-5], or halides of Zn, Pb, Ca, Cd, or Sn. The

effect of compn., vulcanizatin, and fillers on the glass transition, melting and crystn. kinetics of the rubbers was detd.

IT 35277-47-5

CC

(silicone rubber contg., mech. properties of)

RN 35277-47-5 HCA

38 (Elastomers, Including Natural Rubber)

IT 3085-30-1 **35277-47-5**

(silicone rubber contg., mech. properties of)

L38 ANSWER 38 OF 48 HCA COPYRIGHT 1998 ACS

75:110396 Reactions of 8-quinolinol with covalent halides. VI.
Bis-.pi.-cyclopentadienyldihalides of titanium, zirconium, and
hafnium. Frazer, M. J.; Charalambous, J.; Newton, W. E. (Dep.
Chem., North. Polytech., London, Engl.). J. Chem. Soc. A (15),
2487-91 (English) 1971. CODEN: JCSIAP.

The complexes halocyclopentadienyldiquinolin-8-olatometal(IV), C5H5MXox2 (M = Ti, Zr; X = Cl, Br and M = Hf, X = Cl), were prepd. by the direct interaction of quinolin-8-ol (oxH) and dihalobis (cyclopentadienyl)metal (IV) [(C5H5)2MX2] in acetonitrile soln. at room temp. Reactions of these complexes with ethanol, with ethoxide, and H halides were studied. Ir (4000-80 cm-1), NMR, and mass spectra are reported.

IT 34090-33-0P 34765-99-6P

(prepn. of)

RN 34090-33-0 HCA

CN Titanium, chloroethoxybis(8-quinolinolato) - (8CI) (CA INDEX NAME)

RN 34765-99-6 HCA CN Titanium, bromoethoxybis(8-quinolinolato) - (8CI) (CA INDEX NAME)

CC 29 (Organometallic and Organometalloidal Compounds)
IT 34090-33-0P 34765-99-6P
(prepn. of)

L38 ANSWER 39 OF 48 HCA COPYRIGHT 1998 ACS
75:67979 Intramolecular rearrangements in bis(chelate)titanium(IV)
complexes. Harrod, J. F.; Taylor, K. (Chem. Dep., McGill Univ.,

Montreal, Que., Can.). J. Chem. Soc. D. (13), 696-7 (English) 1971.

CODEN: CCJDAO.

The rate of mol. rearrangement of bis(aryloxy)-bis(2,4-pentanedionato)titanium(IV) complexes (aryloxy = XC6H4O, X = p-Me, p-Ac,p-Cl,p-NO2, o-Me, o-iso-Pr, o-I, o-Cl) increases with decreasing pKa of the parent phenol, and the activation entropies for rearrangement are large and neg.

IT 33888-32-3

(nuclear magnetic resonance of, rearrangement in relation to)

RN 33888-32-3 HCA

CN Titanium, bis(2-methyl-8-quinolinolato-N1,08)bis(2-propanolato)-(9CI) (CA INDEX NAME)

IT 23329-69-3

(rearrangement of, kinetics of)

RN 23329-69-3 HCA

CN Titanium, bis(2-propanolato)bis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

67 (Catalysis and Reaction Kinetics) CC 33888-28-7 33888-29-8 33888-26-5 33888-27-6 IT33888-25-4 33888-31-2 **33888-32-3** 33888-33-4 33888-30-1 33939-16-1 (nuclear magnetic resonance of, rearrangement in relation to) 21324-45-8 23329-69-3 33887-44-4 TI 17927-72-9 33887-48-8 33887-49-9 33887-46-6 33887-47-7 33887-45-5 33887-50-2 33888-34-5 (rearrangement of, kinetics of)

L38 ANSWER 40 OF 48 HCA COPYRIGHT 1998 ACS
75:64782 Effectiveness of some poly(dimethylsiloxane) stabilizers.
Ditsent, V. E.; Skorokhodov, I. I.; Terent'eva, N. A.; Zolotareva,
M. N. (USSR). Sin. Issled. Eff. Khimikatov Polim. Mater., No. 3,
192-8 From: Ref. Zh., Khim. 1970, Abstr. No. 118808 (Russian) 1969.

Twenty-four classes of compds. were studied as stabilizers against thermal oxidative breakdown of .omega.,.omega.'hexamethyloligodimethylsiloxane. Organosilicone derivs. of ferrocene, cyclopentadienylbenzoyltricarbonylmanganese and its derivs., bis(8-hydroxyquinoline)dibutoxytitanium, and 4,4-dimethoxydiphenylamine are the most effective stabilizers, which makes possible an increase of 60-70.degree. in the incipient thermal-oxidative breakdown temp. of oligodimethylsiloxane.

IT 17034-82-1

(stabilizers, for siloxanes)

RN 17034-82-1 HCA

CN Titanium, dibutoxybis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

CC 36 (Plastics Manufacture and Processing)
IT 101-70-2 17034-82-1 33306-83-1
(stabilizers, for siloxanes)

L38 ANSWER 41 OF 48 HCA COPYRIGHT 1998 ACS
73:114013 Crystal and molecular structure of chloro-.pi.cyclopentadienylbis(8-quinolinolato)titanium(IV). Matthews, James
D.; Singer, N.; Swallow, Arnold G. (Dep. Chem., Northern Polytech.,
London, Engl.). J. Chem. Soc. A (15), 2545-9 (English) 1970.
CODEN: JCSIAP.

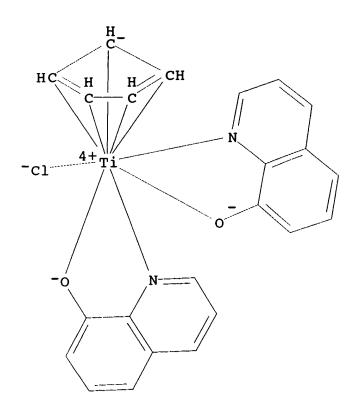
The crystal and mol. structure of [TiCl(.pi.-C5H5)(C9H6NO)2] has been detd. from 3-dimensional x-ray diffraction data. The unit cell is monoclinic with a = 8.82, b = 13.85, c = 16.80 .ANG., .beta. = 111.7.degree., and space group P21/c. The structure was solved by Patterson and Fourier methods from 2402 independent visually estd. intensities and refined by least-squares to R 0.098. The structure consists of monomeric units with mol. geometry best described as dodecahedral but with certain similarities to a distorted octahedron. The O atoms lie in a trans-configuration, with respect to the octahedron, at 1.987 and 1.954 from the Ti, the N atoms cis at 2.224 and 2.270, and the Cl atom at 2.372 .ANG.. The long Ti-Cl distance and the differences between the Ti-O and Ti-N distances are discussed and compared with the corresponding distances in related compds.

IT 31798-62-6

(crystal structure of)

RN 31798-62-6 HCA

CN Titanium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(8-quinolinolato-N1,08)-, stereoisomer (9CI) (CA INDEX NAME)



CC 70 (Crystallization and Crystal Structure)
IT 31798-62-6
(crystal structure of)

L38 ANSWER 42 OF 48 HCA COPYRIGHT 1998 ACS
70:68818 Poly[bis(8-quinolinoxy)titanoxymethylphenylsiloxanes].
Zhinkina, L. N.; Severnyi, V. V.; Altukhova, T. F. (USSR). Plast.
Massy (1), 26-9 (Russian) 1969. CODEN: PLMSAI.

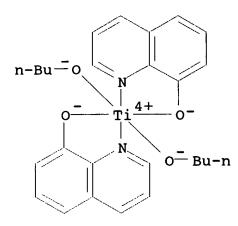
The effect was studied of bis(8-quinolinoxy)titanium unit content on the properties of the title polymers (I), prepd. by polycondensation of poly(methylphenysiloxanol) contg. 3-4% OH groups with bis(8-quinolinoxy)dibutoxytitanium (II). I having Si-Ti ratios of 10, 50, 100, 200, 400, and 800 were obtained. Oxidative thermal stability of I films was studied. Thermogravimetric and differential curves of I are recorded. Adhesion and dielec. properties of I were also detd. The treatment of low-mol.-wt. poly(organosiloxanols) with II allows the prepn. of polymers with improved properties while avoiding alk. and oxidative condensation.

IT 17034-82-1P

(polymers with hydroxy-terminated methylphenylsiloxanes, prepn. of)

RN 17034-82-1 HCA

CN Titanium, dibutoxybis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)



CC 35 (Synthetic High Polymers)

IT 17034-82-1P

(polymers with hydroxy-terminated methylphenylsiloxanes, prepn. of)

L38 ANSWER 43 OF 48 HCA COPYRIGHT 1998 ACS

70:53556 Titanium(IV) complexes with 8-quinolinol. Sen, D. N.;
Umapathy, P. (Nat. Chem. Lab., Poona, India). J. Indian Chem. Soc.,
45(11), 1006-11 (English) 1968. CODEN: JICSAH.

Ti(OR)2L2, where R = Et, iso-Pr, Bu, and HL = 8-quinolinol, were prepd. and studied. Titanoxane polymers were obtained by the hydrolysis of Ti(OR)2L2 and of the reaction product of TiCl4 with 8-quinolinol. Absorption bands due to alkoxy groups were absent in the ir spectra of the hydrolysis products of the dialkoxy compds. Strong and broad bands at .apprx.825 cm.-1 and at .apprx.735 cm.-1 ascribable to Ti-O-Ti stretching frequency were observed in the spectra of the hydrolysis products.

IT 17034-82-1P 23329-68-2P 23329-69-3P

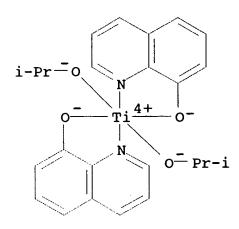
(prepn. of)

RN 17034-82-1 HCA

CN Titanium, dibutoxybis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

RN 23329-68-2 HCA CN Titanium, diethoxybis(8-quinolinolato-N1,02)- (9CI) (CA INDEX NAME)

RN 23329-69-3 HCA CN Titanium, bis(2-propanolato)bis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)



CC 78 (Inorganic Chemicals and Reactions)
IT 17034-82-1P 22967-16-4P 22967-17-5P 23329-68-2P
23329-69-3P
(prepn. of)

L38 ANSWER 44 OF 48 HCA COPYRIGHT 1998 ACS
69:62437 Crystal and molecular structure of dichlorobis(8quinolinolato)titanium(IV). Studd, B. F.; Swallow, A. G. (Dep.
Chem., Northern Polytech., London, Engl.). J. Chem. Soc., A (8),
1961-7 (English) 1968. CODEN: JCSIAP.

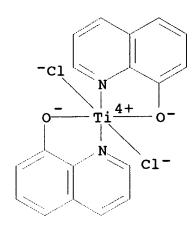
The crystal and mol. structure of TiCl2(C9H6NO)2 has been detd. by three-dimensional x-ray diffraction. The unit cell is monoclinic with a = 14.06, b = 8.54, c = 14.97 A., .beta. = 111.degree., and space group C2/c. The structure was solved by use of 1415 visually estd. intensities by Patterson and Fourier methods and refined by least sqs. to an R value of 0.116. The structure consists of monomeric units of TiCl2(Ox)2, with two-fold symmetry, in which the Ti atom is octahedrally coordinated by two Cl atoms in a cis configuration, at a distance of 2.283, two N atoms also cis at 2.200, and two oxygen atoms in a trans configuration at 1.888 A. The large difference between the Ti-N and Ti-O distance is discussed and compared with distances in other metal-oxine complexes. 17 references.

IT 16905-40-1

(structure of)

RN 16905-40-1 HCA

CN Titanium, dichlorobis(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)



CC 70 (Crystallization and Crystal Structure)
IT 16905-40-1

(structure of)

L38 ANSWER 45 OF 48 HCA COPYRIGHT 1998 ACS

68:117788 Structure of dichlorodi-8-quinolinolatotitanium(IV). Swallow, Arnold G.; Studd, B. F. (Chem. Dep., Northern Polytech., London, Engl.). Chem. Commun. (23), 1197-8 (English) 1967. CODEN: CCOMA8.

8-Quinolinol (QOH) is treated with TiCl4 (TiCl4:QOH molar ratio 1:2) to give TiCl4.2QOH (I); HCl is removed from I to give the title compd. (II), with a 14.06, b 8.54, c 14.97 A., .beta. 111.degree. space group C2/c; dm is 1.64 and dc 1.61, Z = 4. II has a crystallographic 2-fold axis through the Ti atom, bisecting the Cl-Ti-Cl angle (97.degree.) and the N-Ti-N angle.

IT 16905-40-1

(crystal structure of)

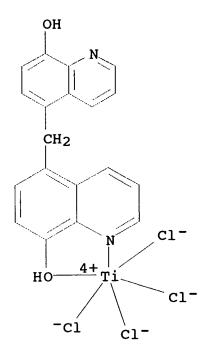
RN 16905-40-1 HCA

CN Titanium, dichlorobis(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)

```
70 (Crystallization and Crystal Structure)
IT 16905-40-1
        (crystal structure of)
    ANSWER 46 OF 48 HCA COPYRIGHT 1998 ACS
67:82436 Coordination polymers of titanium(IV), tin(IV), and
                     Sen, Dwijendra N.; Umapathy, P. (Natl. Chem. Lab.,
     zirconium(IV).
                     Indian J. Chem., 5(5), 209-10 (English) 1967.
     Poona, India).
     CODEN: IJOCAP.
     The polymers were prepd. by adding TiCl4, Ti(OBu)4, Me2SnCl2, and
AB
     ZrOC12.8H2O to heated solns. of bis(8-hydroxy-5-quinoly1) methane in
               Decompn. temps. for the Ti(IV), Zr(IV), and Sn(IV)
     polymers were 330.degree., 380.degree., and 410.degree., resp.,
     indicating that thermal stability increased with at. no. of the
            The polymer yields were 52.36, 97.5, 52.9, and 70%, resp.,
     for TiCl4, Ti(OBu)4, Me2SnCl2, and ZrOCl2.
IT 30972-50-0P
        (prepn. of)
     30972-50-0 HCA
RN
     8-Quinolinol, 5,5'-methylenedi-, polymer with titanium chloride
CN
     (TiCl3) (8CI) (CA INDEX NAME)
```

CM 1

CRN 52928-48-0 CMF C19 H14 C14 N2 O2 Ti CCI CCS CDES 7:OC-6-32



CC 35 (Synthetic High Polymers)
IT 30972-50-0P 30972-51-1P 31114-18-8P (prepn. of)

ANSWER 47 OF 48 HCA COPYRIGHT 1998 ACS L38 66:76121 Chemical transformations of dizirconoxane compounds. Freidlina, R. Kh.; Brainina, E. M.; Petrashkevich, L. A.; Minacheva, Izv. Akad. Nauk M. Kh. (Inst. Hetero-Org. Compds., Moscow, USSR). SSSR, Ser. Khim. (8), 1396-9 (Russian) 1966. CODEN: IASKA6. cf. CA 60, 12038g. Heating 0.018 g. H2O, 0.0896 g. abs. EtOH, 0.197 AB g. Et3N, 1.0 g. dibenzoylacetonatocyclopentadienylzirconium chloride and C6H6 1 hr. at 40-5.degree. gave after sepn. of Et3N.HCl 64% dicyclopentadienyldizirconoxane tetrabenzoylacetonate (I), [(C5H5)(C10H9O2)2Zr]2O, decompd. at 172-5.degree., which contained stubbornyl held C6H6. Similar reaction with bis - 8 hydroxyquinolinocyclopentadienylzirconium chloride (prepd. from (C5H5)2ZrCl2 and 8-hydroxyqinoline in C6H6, m. 260-3.degree.), gave dicyclopentadienyldizirconoxane tetra-8-hydroxyquinolinate (II), [(C5H5)(C9H6ON)2Zr]2O, infusible at 300.degree.. Adding p-MeC6H4SO3H in tetrahydrofuran to [(C5H5)2ZrCl]20 at 5.degree. gave in 2 hrs. 50% (C5H5)2ZrCl(O3SC6H4Me-p).H2O, m. 166-9.degree.; similar reaction with concd. H2SO4 in (CH2Cl)2 gave 62% (C5H5)2Zr(OSO3H)2.4H2O, infusible and hygroscopic solid; similarly HNO3 gave (C5H5)2ZrClNO3, m. 190.5.degree.. Reaction of HNO3 (d. 135) in (CH2Cl)2 with dicyclopentadienylzirconium dichloride at -30.degree., followed by 1 hr. at room temp., gave 62% (C5H5)2ZrCl(NO3), m. 190.degree., as above. Reaction of



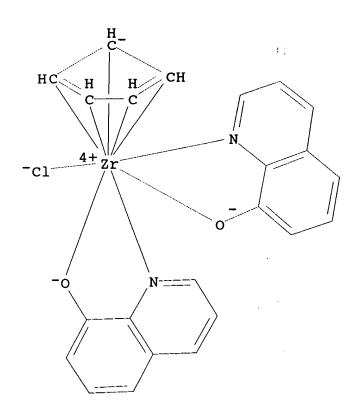
p-MeC6H4SO3H with dicyclopentadienyldizirconoxane tetraacetyl-acetonate in tetrahydrofuran, finally at 40.degree., gave 77% (C5H5) (C5H7O2)2Zr(O3SC6H4Me-p).0.5C4H8O, m.
187.5-90.degree. (from tetrahydrofuran); HNO3 similarly gave 47% (C5H5)(C5H7O2)2Zr(NO3), m. 137-40.degree. Heating CH2Bz2 with tetracyclopentadienyldizirconoxane dichloride at 100-10.degree. 40 min. gave 45% (C15H11O2)2ZrCl(C5H5) decompd. at 225-7.degree.; similarly 8-hydroxyquinoline gave (C9H6ON)2ZrCl(C5H5), m.
260-3.degree.. Bz2CH2 and (C5H5)2ZrCl2 at 90.degree. in C6H6 in vacuo 22 hrs. gave 65% bis(dibenzoylmethanocyclopentadienyl)zirconium chloride, decompd. at 224-6.degree.; similar reaction with 8-hydroxyquinoline gave 76% bis(8-hydroxyquinolinate) of cyclopentadienylzirconium chloride, (C9H6ON)2ZrCl(C5H5), m.
260-3.degree.. The above reactions illustrated the basic nature of the dizirconoxane group.

IT 12114-15-7P

(prepn. of)

RN 12114-15-7 HCA

CN Zirconium, chloro(.eta.5-2,4-cyclopentadien-1-yl)bis(8-quinolinolato-N1,08)-, stereoisomer (9CI) (CA INDEX NAME)



CC 29 (Organometallic and Organometalloidal Compounds)
IT 12111-83-0P 12114-03-3P **12114-15-7P** 12116-65-3P
12119-26-5P 12121-09-4P 12124-07-1P 12193-45-2P 12193-84-9P
(prepn. of)

L38 ANSWER 48 OF 48 HCA COPYRIGHT 1998 ACS

66:70504 Far infrared spectra of some compounds of Group IV tetrahalides with 8-quinolinol, salicylaldehyde, and acetylacetone. Douek, I.; Frazer, Malcolm J.; Goffer, Z.; Goldstein, Michael; Rimmer, B.; Willis, Harry A. (Northern Polytech., London, Engl.). Spectrochim. Acta, 23A(2), 373-81 (English) 1967. CODEN: SPACA5.

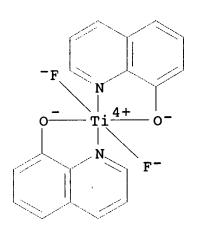
The far ir spectra (450-80 cm.-1) of several complexes of the type MX2ke2, MX4.2keH, and MX4.keH (M = Ti, Zr, Ge, or Sn; X = F, Cl, Br, or I; keH = 8-quinolinol, salicylaldehyde, or acetylacetone) have been studied. Vibrations involving metal-halogen stretching have been assigned, and suggestions made as to the likely stereochem. configurations of some of the compds., but because of the complexity of the spectra and other factors discussed, it has not been possible to establish configurations unequivocally. Possibly the complexes TiCl4.(8-quinolinol) and SnCl4.(8-quinolinol) are monomeric, 5-coordinate species in the solid state. For analogous compds., the relation .nu.(SnX)/.nu.(TiX) .apprx.0.90 is independent of the halogen and other ligands, and applies to all the compds. now studied as well as to those previously reported in the literature. 37 references.

IT 16905-21-8 16905-40-1 19032-85-0 19049-15-1 19381-58-9

(spectrum (ir) of)

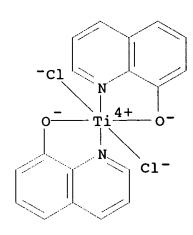
RN 16905-21-8 HCA

CN Titanium, difluorobis(8-quinolinolato-N1,08)- (9CI) (CA INDEX NAME)

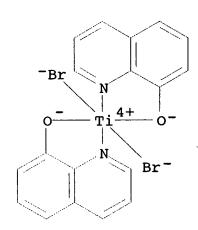


RN 16905-40-1 HCA

CN Titanium, dichlorobis(8-quinolinolato-.kappa.N1,.kappa.O8)- (9CI) (CA INDEX NAME)



RN 19032-85-0 HCA CN Titanium, dibromobis(8-quinolinolato)-, trans- (8CI) (CA INDEX NAME)



RN 19049-15-1 HCA CN Titanium, tetrafluorobis(8-quinolinol)- (8CI) (CA INDEX NAME)

RN 19381-58-9 HCA CN Zirconium, tetrachlorobis(8-quinolinol)- (8CI) (CA INDEX NAME)

CC 73 (Spectra and Other Optical Properties)
IT 148-24-3, properties 15523-68-9 16905-21-8 16905-24-1

Page 153

Rabago 08/872,659

16905-25-2	16905-26-3	16905-27-4	16905-35-4	16905-40-1
16905-42-3	16919-65-6	16919-66-7	16919-67-8	16925-43-2
17029-26-4	17099-86-4	17185-49-8	17218-25-6	19032-85-0
19049-15-1	19154-04-2	19154-08-6	19154-09-7	
19154-10-0	19154-11-1	19154-12-2	19154-13-3	19154-16-6
19154-17-7	19381-58-9	19978-93-9		
(spectri	ım (ir) of)			